



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 03:59 PM EDT

PDB ID : 3RI5  
Title : C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab, ivermectin and picrotoxin  
Authors : Hibbs, R.E.; Gouaux, E.  
Deposited on : 2011-04-12  
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

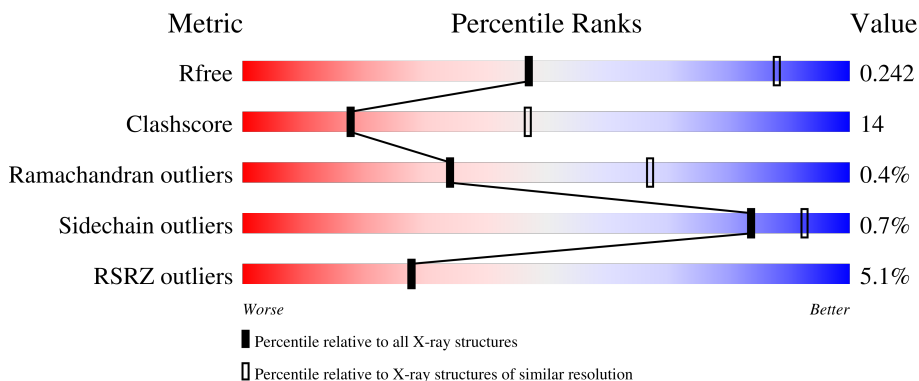
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



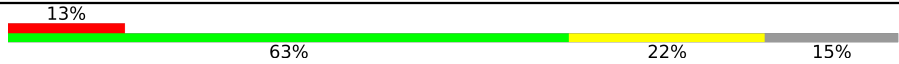
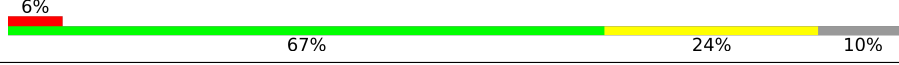

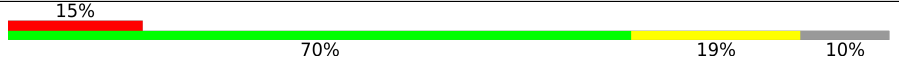
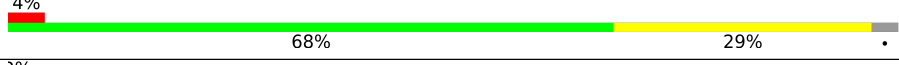
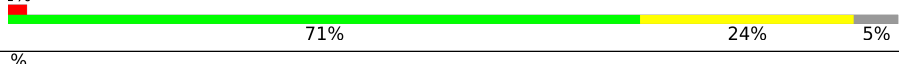


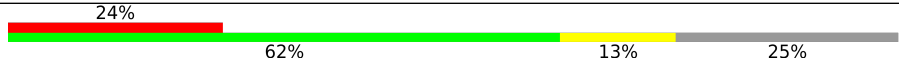

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	69% 28% ..
1	B	347	68% 29% ..
1	C	347	69% 28% ..
1	D	347	68% 29% ..
1	E	347	68% 29% ..

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Mol	Chain	Length	Quality of chain
2	F	221	
2	G	221	
2	H	221	
2	I	221	
2	J	221	
3	K	210	
3	L	210	
3	M	210	
3	N	210	
3	O	210	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	RI5	E	351	-	-	X	-
5	LMT	A	351	-	-	-	X
5	LMT	B	350	-	-	-	X
7	OCT	D	350	-	-	-	X
7	OCT	E	350	-	-	-	X
8	UND	B	352	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 29167 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Avermectin-sensitive glutamate-gated chloride channel GluCl alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2716	1768	441	492	15	0	0	0
1	B	340	2716	1768	441	492	15	0	0	0
1	C	339	2706	1762	438	491	15	0	0	0
1	D	340	2716	1768	441	492	15	0	0	0
1	E	340	2716	1768	441	492	15	0	0	0

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	ALA	-	linker	UNP O17793
A	304	GLY	-	linker	UNP O17793
A	305	THR	-	linker	UNP O17793
A	340	HIS	-	expression tag	UNP O17793
A	341	HIS	-	expression tag	UNP O17793
A	342	HIS	-	expression tag	UNP O17793
A	343	HIS	-	expression tag	UNP O17793
A	344	HIS	-	expression tag	UNP O17793
A	345	HIS	-	expression tag	UNP O17793
A	346	HIS	-	expression tag	UNP O17793
A	347	HIS	-	expression tag	UNP O17793
B	303	ALA	-	linker	UNP O17793
B	304	GLY	-	linker	UNP O17793
B	305	THR	-	linker	UNP O17793
B	340	HIS	-	expression tag	UNP O17793
B	341	HIS	-	expression tag	UNP O17793
B	342	HIS	-	expression tag	UNP O17793
B	343	HIS	-	expression tag	UNP O17793

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Chain	Residue	Modelled	Actual	Comment	Reference
B	344	HIS	-	expression tag	UNP O17793
B	345	HIS	-	expression tag	UNP O17793
B	346	HIS	-	expression tag	UNP O17793
B	347	HIS	-	expression tag	UNP O17793
C	303	ALA	-	linker	UNP O17793
C	304	GLY	-	linker	UNP O17793
C	305	THR	-	linker	UNP O17793
C	340	HIS	-	expression tag	UNP O17793
C	341	HIS	-	expression tag	UNP O17793
C	342	HIS	-	expression tag	UNP O17793
C	343	HIS	-	expression tag	UNP O17793
C	344	HIS	-	expression tag	UNP O17793
C	345	HIS	-	expression tag	UNP O17793
C	346	HIS	-	expression tag	UNP O17793
C	347	HIS	-	expression tag	UNP O17793
D	303	ALA	-	linker	UNP O17793
D	304	GLY	-	linker	UNP O17793
D	305	THR	-	linker	UNP O17793
D	340	HIS	-	expression tag	UNP O17793
D	341	HIS	-	expression tag	UNP O17793
D	342	HIS	-	expression tag	UNP O17793
D	343	HIS	-	expression tag	UNP O17793
D	344	HIS	-	expression tag	UNP O17793
D	345	HIS	-	expression tag	UNP O17793
D	346	HIS	-	expression tag	UNP O17793
D	347	HIS	-	expression tag	UNP O17793
E	303	ALA	-	linker	UNP O17793
E	304	GLY	-	linker	UNP O17793
E	305	THR	-	linker	UNP O17793
E	340	HIS	-	expression tag	UNP O17793
E	341	HIS	-	expression tag	UNP O17793
E	342	HIS	-	expression tag	UNP O17793
E	343	HIS	-	expression tag	UNP O17793
E	344	HIS	-	expression tag	UNP O17793
E	345	HIS	-	expression tag	UNP O17793
E	346	HIS	-	expression tag	UNP O17793
E	347	HIS	-	expression tag	UNP O17793

- Molecule 2 is a protein called Mouse monoclonal Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	188	1441	915	234	285	7	0	0	0

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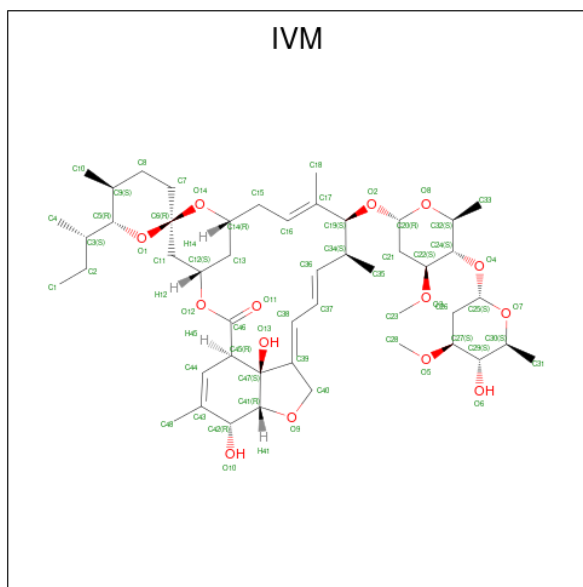
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	200	Total	C	N	O	S	0	0	0
			1529	973	248	301	7			
2	H	221	Total	C	N	O	S	0	0	0
			1683	1067	273	335	8			
2	I	199	Total	C	N	O	S	0	0	0
			1525	969	247	301	8			
2	J	215	Total	C	N	O	S	0	0	0
			1639	1043	265	324	7			

- Molecule 3 is a protein called Mouse monoclonal Fab fragment, light chain.

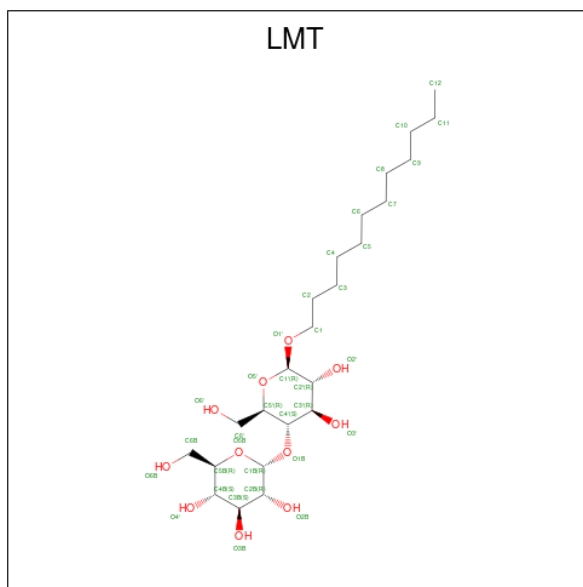
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	199	Total	C	N	O	S	0	0	0
			1496	941	246	303	6			
3	L	210	Total	C	N	O	S	0	0	0
			1591	999	266	320	6			
3	M	210	Total	C	N	O	S	0	0	0
			1579	993	261	319	6			
3	N	158	Total	C	N	O	S	0	0	0
			1156	728	192	233	3			
3	O	195	Total	C	N	O	S	0	0	0
			1470	927	243	294	6			

- Molecule 4 is (2aE,4E,5'S,6S,6'R,7S,8E,11R,13R,15S,17aR,20R,20aR,20bS)-6'-[(2S)-butan-2-yl]-20,20b-dihydroxy-5',6,8,19-tetramethyl-17-oxo-3',4',5',6,6',10,11,14,15,17,17a,20,20a,20b-tetradecahydro-2H,7H-spiro[11,15-methanofuro[4,3,2-pq][2,6]benzodioxacy cloctadecine-1,3,2'-pyran]-7-yl 2,6-dideoxy-4-O-(2,6-dideoxy-3-O-methyl-alpha-L-arabino-hexopyranosyl)-3-O-methyl-alpha-L-arabino-hexopyranoside (three-letter code: IVM) (formula: C<sub>48</sub>H<sub>74</sub>O<sub>14</sub>).



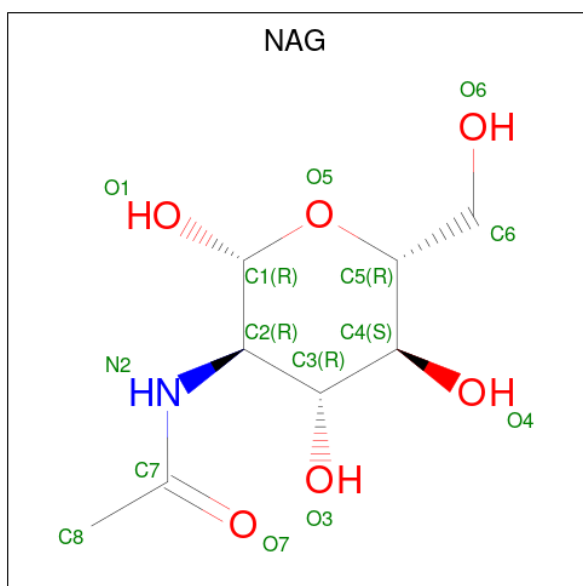
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 62 48 14	0	0
4	B	1	Total C O 62 48 14	0	0
4	C	1	Total C O 62 48 14	0	0
4	D	1	Total C O 62 48 14	0	0
4	E	1	Total C O 62 48 14	0	0

- Molecule 5 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 26 15 11	0	0
5	A	1	Total C O 27 16 11	0	0
5	B	1	Total C O 26 15 11	0	0

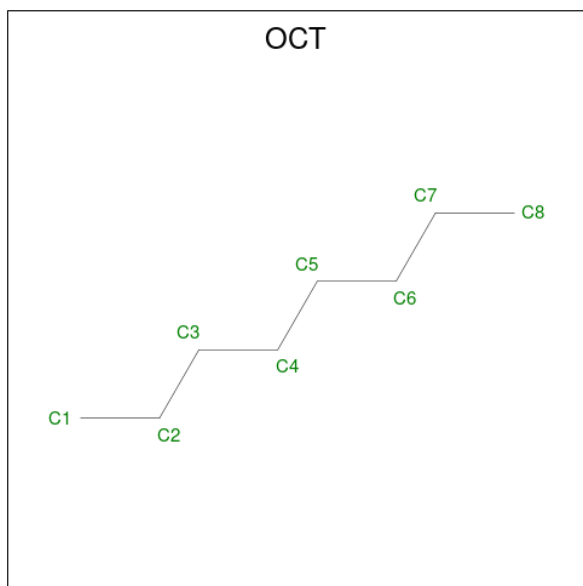
- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





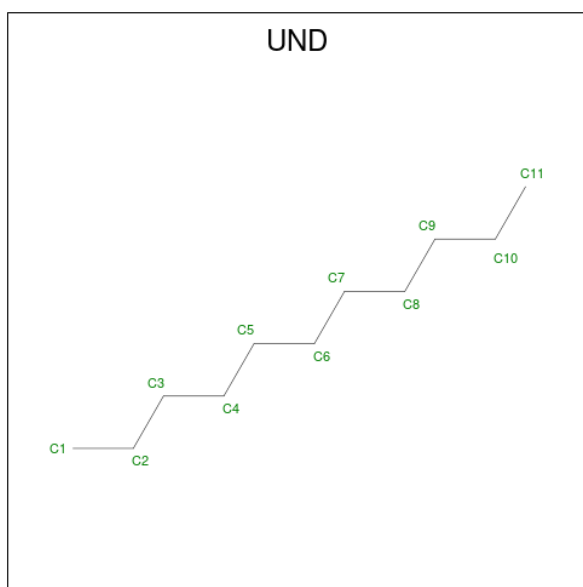
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is N-OCTANE (three-letter code: OCT) (formula: C<sub>8</sub>H<sub>18</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	C	0	0
			8	8		
7	D	1	Total	C	0	0
			8	8		
7	E	1	Total	C	0	0
			8	8		

- Molecule 8 is UNDECANE (three-letter code: UND) (formula: C<sub>11</sub>H<sub>24</sub>).

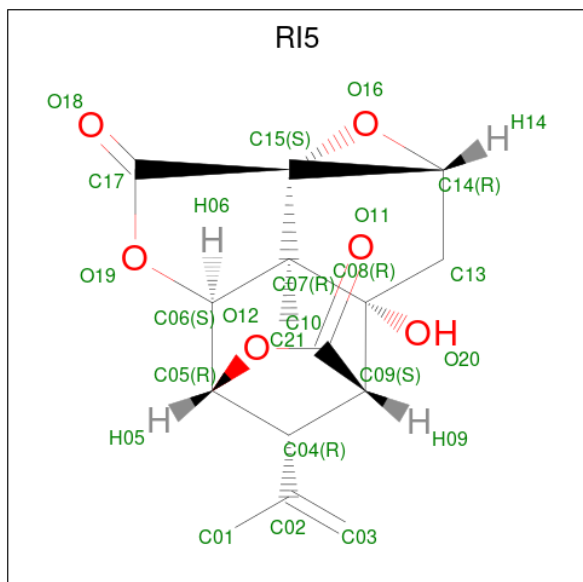


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 11 11	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Cl 1 1	0	0

- Molecule 10 is (1aR,2aR,3S,6R,6aS,8aS,8bR,9R)-2a-hydroxy-8b-methyl-9-(prop-1-en-2-yl)hexahydro-3,6-methano-1,5,7-trioxacyclopenta[ij]c yclopropa[a]azulene-4,8(3H)-dione (three-letter code: RI5) (formula: C<sub>15</sub>H<sub>16</sub>O<sub>6</sub>).

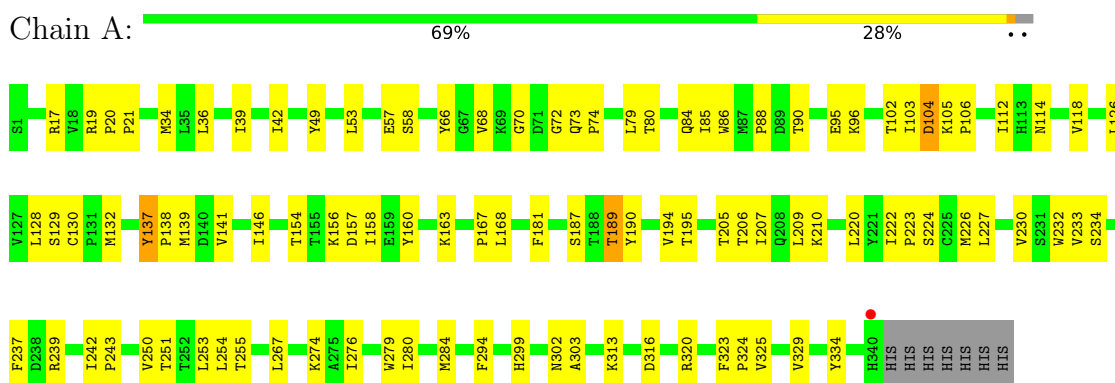


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	E	1	21	15	6	0	0

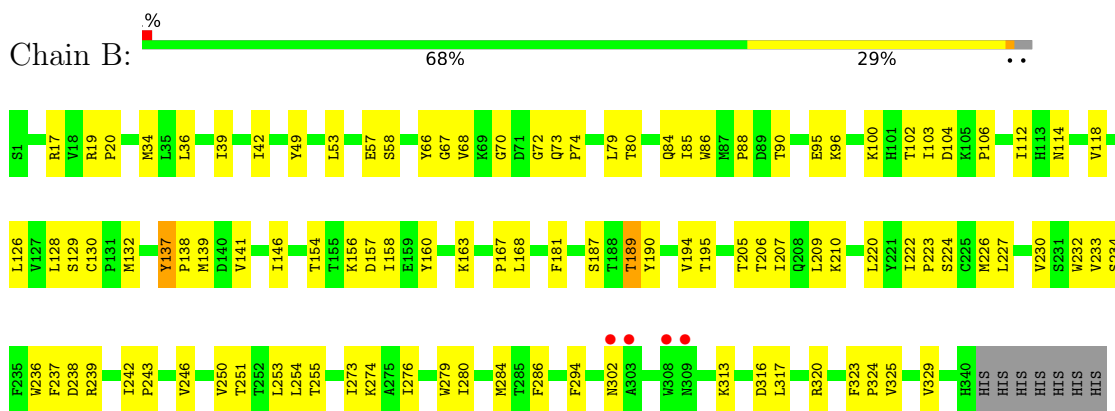
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

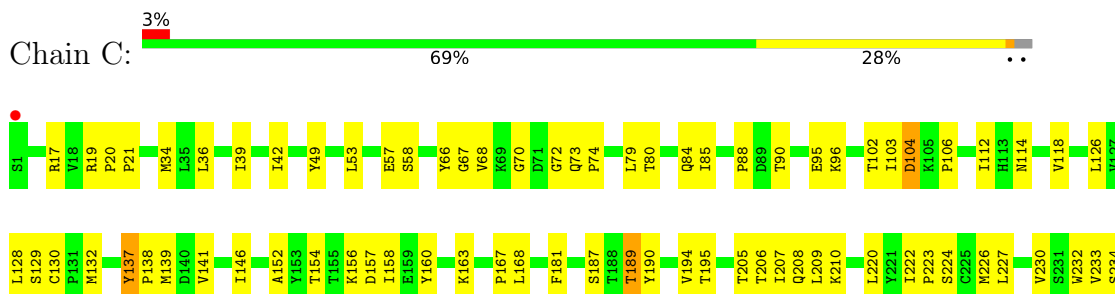
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

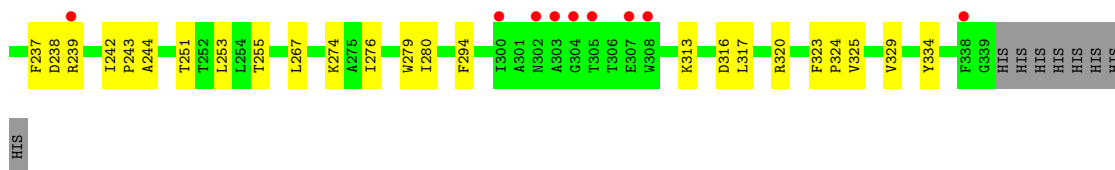


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



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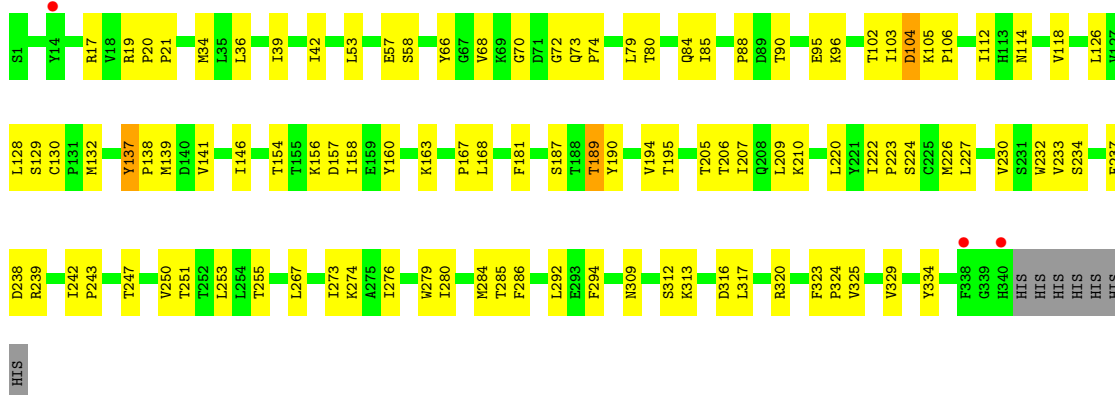




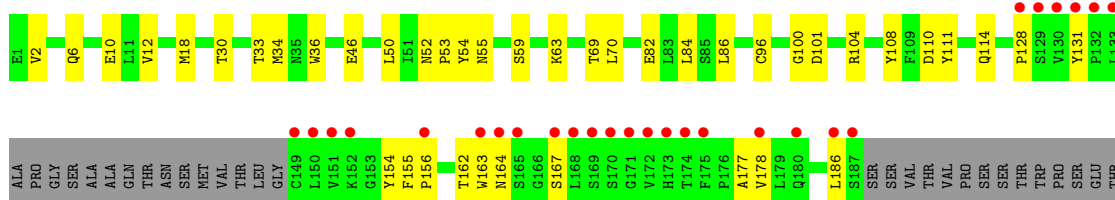
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



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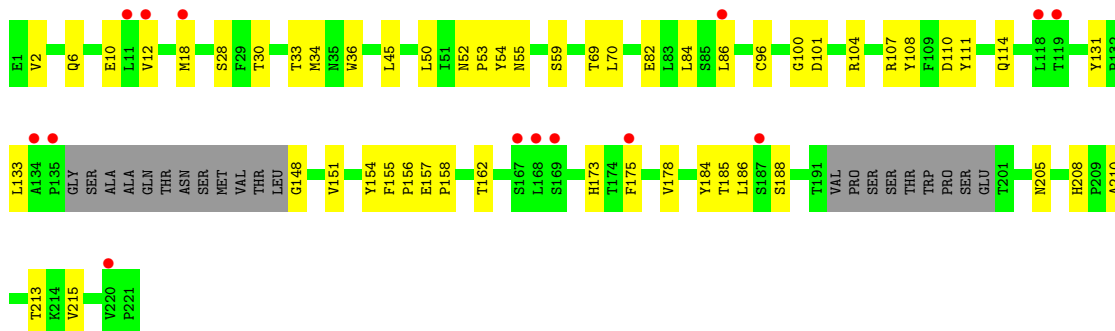


• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

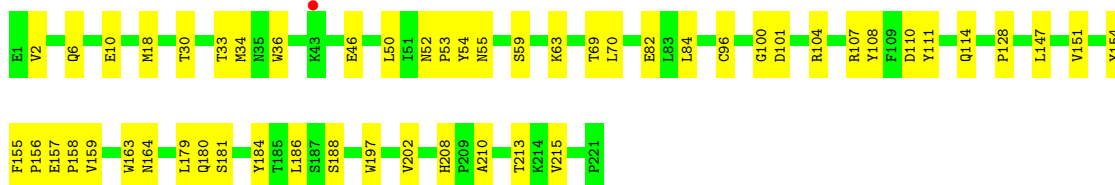
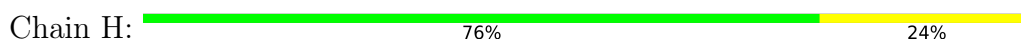




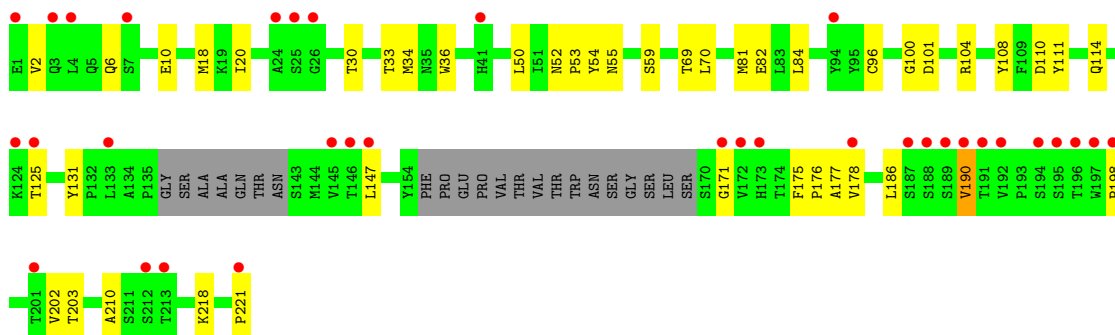
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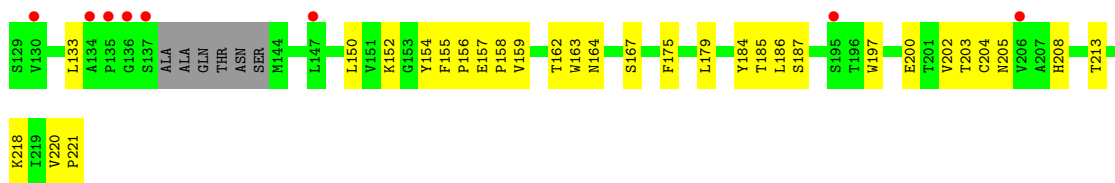


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

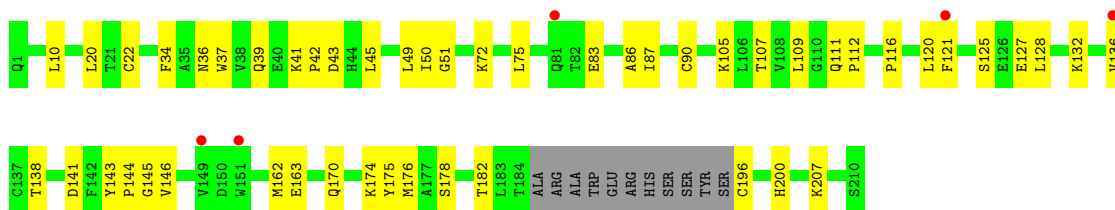


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

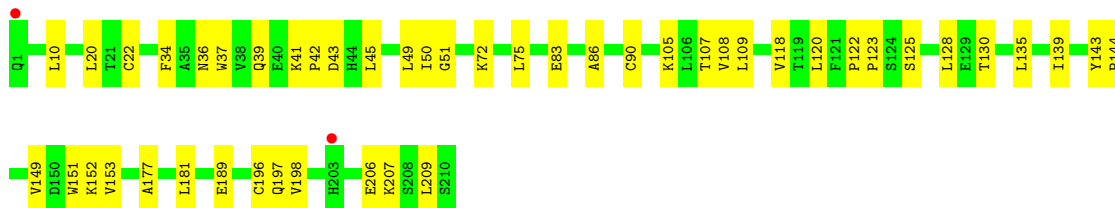
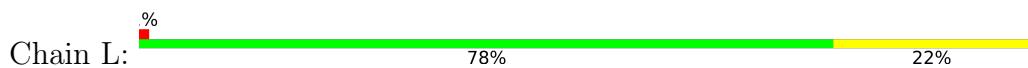




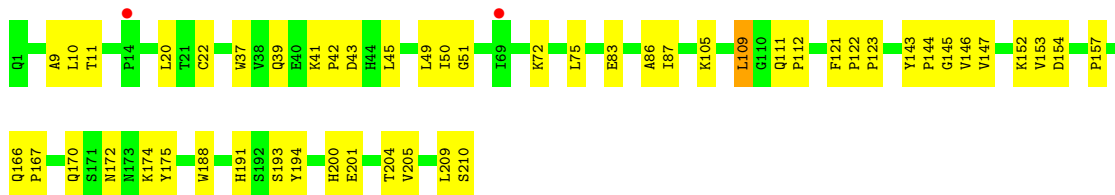
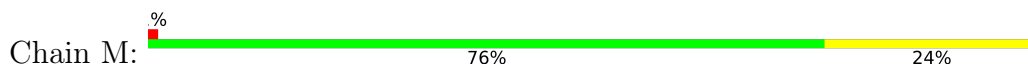
- Molecule 3: Mouse monoclonal Fab fragment, light chain



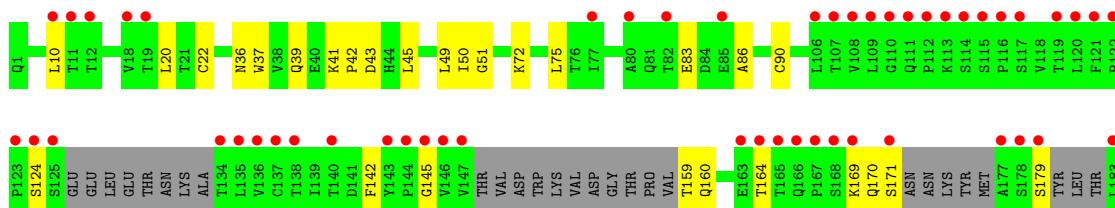
- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain




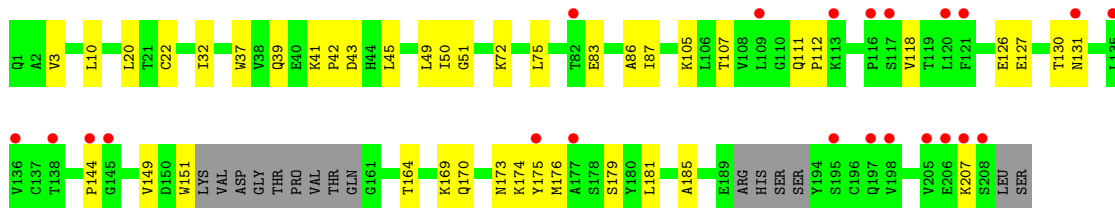
- Molecule 3: Mouse monoclonal Fab fragment, light chain



T184  
A185  
ARG  
ALA  
TRP  
GLU  
ARG  
HIS  
SER  
SER  
TYR  
SER  
CYS  
GLN  
VAL  
THR  
HIS  
GLU  
GLY  
HIS  
THR  
VAL  
GLU  
LYS  
SER  
LEU  
SER

- Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain O:  10% 73% 20% 7%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.84Å 154.84Å 573.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 3.40 49.83 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.83-3.40) 98.8 (49.83-3.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 3.40Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.232 , 0.248 0.226 , 0.242	Depositor DCC
$R_{free}$ test set	4809 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.8	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	29167	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IVM, CL, OCT, RI5, UND, NAG, LMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/2789	0.41	0/3809
1	B	0.25	0/2789	0.40	0/3809
1	C	0.24	0/2778	0.40	0/3794
1	D	0.24	0/2789	0.40	0/3809
1	E	0.24	0/2789	0.40	0/3809
2	F	0.23	0/1479	0.40	0/2014
2	G	0.25	0/1569	0.44	0/2138
2	H	0.24	0/1729	0.42	0/2360
2	I	0.22	0/1564	0.41	0/2128
2	J	0.23	0/1684	0.42	0/2299
3	K	0.22	0/1529	0.42	0/2089
3	L	0.24	0/1629	0.42	0/2226
3	M	0.22	0/1616	0.42	0/2211
3	N	0.22	0/1178	0.42	0/1609
3	O	0.22	0/1504	0.43	0/2056
All	All	0.24	0/29415	0.41	0/40160

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2716	0	2709	101	0
1	B	2716	0	2708	98	0
1	C	2706	0	2701	93	0
1	D	2716	0	2709	93	0
1	E	2716	0	2708	103	0
2	F	1441	0	1365	35	0
2	G	1529	0	1478	43	0
2	H	1683	0	1632	43	0
2	I	1525	0	1485	35	0
2	J	1639	0	1588	48	0
3	K	1496	0	1458	35	0
3	L	1591	0	1542	32	0
3	M	1579	0	1526	37	0
3	N	1156	0	1128	20	0
3	O	1470	0	1412	35	0
4	A	62	0	74	5	0
4	B	62	0	74	2	0
4	C	62	0	74	5	0
4	D	62	0	74	3	0
4	E	62	0	74	7	0
5	A	53	0	52	14	0
5	B	26	0	25	5	0
6	B	14	0	13	1	0
6	C	14	0	13	1	0
6	E	14	0	13	0	0
7	B	8	0	18	1	0
7	D	8	0	18	1	0
7	E	8	0	18	3	0
8	B	11	0	24	0	0
9	C	1	0	0	0	0
10	E	21	0	16	15	0
All	All	29167	0	28729	786	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (786) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:HIS:CD2	5:A:350:LMT:H12	1.79	1.17
1:A:299:HIS:HD2	5:A:350:LMT:H12	0.96	1.08
1:A:299:HIS:CD2	5:A:350:LMT:C1	2.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:THR:OG1	10:E:351:RI5:H13	1.57	1.01
1:A:299:HIS:HD2	5:A:350:LMT:C1	1.73	0.99
3:L:107:THR:HG21	3:L:144:PRO:HB3	1.45	0.98
1:D:195:THR:HA	2:I:55:ASN:ND2	1.83	0.93
1:C:90:THR:HG22	1:C:160:TYR:OH	1.70	0.92
1:D:90:THR:HG22	1:D:160:TYR:OH	1.70	0.92
1:B:90:THR:HG22	1:B:160:TYR:OH	1.70	0.91
1:A:90:THR:HG22	1:A:160:TYR:OH	1.71	0.90
1:B:195:THR:HA	2:F:55:ASN:ND2	1.85	0.90
1:E:243:PRO:CB	10:E:351:RI5:H03	2.02	0.90
1:E:90:THR:HG22	1:E:160:TYR:OH	1.71	0.89
1:E:243:PRO:HB3	10:E:351:RI5:C03	2.03	0.89
1:E:243:PRO:HB3	10:E:351:RI5:H03	1.57	0.87
1:A:243:PRO:HB3	10:E:351:RI5:H01B	1.55	0.86
1:E:195:THR:HA	2:J:55:ASN:ND2	1.91	0.84
1:B:195:THR:HA	2:F:55:ASN:HD21	1.46	0.80
1:E:243:PRO:CB	10:E:351:RI5:C03	2.62	0.78
1:D:195:THR:HA	2:I:55:ASN:HD21	1.45	0.77
1:C:208:GLN:HB2	6:C:400:NAG:H82	1.67	0.77
1:A:195:THR:HA	2:H:55:ASN:ND2	2.01	0.76
1:A:253:LEU:HD11	1:B:226:MET:HE1	1.68	0.75
1:D:243:PRO:HB3	10:E:351:RI5:H03A	1.70	0.74
1:B:236:TRP:CH2	5:B:350:LMT:H12	2.23	0.73
3:L:120:LEU:HD12	3:L:196:CYS:HB3	1.69	0.73
3:L:139:ILE:HD12	3:L:198:VAL:HG21	1.68	0.73
1:B:253:LEU:HD11	1:C:226:MET:HE1	1.70	0.73
2:J:128:PRO:HB3	2:J:154:TYR:HB3	1.69	0.73
3:L:152:LYS:HD3	3:L:197:GLN:NE2	2.03	0.73
1:C:17:ARG:HB3	1:D:80:THR:HB	1.72	0.72
1:A:299:HIS:CD2	5:A:350:LMT:H11	2.24	0.72
1:C:195:THR:HA	2:G:55:ASN:ND2	2.05	0.71
1:C:226:MET:HG3	4:C:350:IVM:H11A	1.71	0.71
1:B:253:LEU:HD11	1:C:226:MET:CE	2.20	0.71
1:A:253:LEU:HD11	1:B:226:MET:CE	2.21	0.70
3:L:125:SER:HA	3:L:128:LEU:HD12	1.72	0.70
2:J:164:ASN:HB2	2:J:167:SER:HB3	1.74	0.70
1:A:243:PRO:CB	10:E:351:RI5:H01B	2.22	0.70
1:D:224:SER:HB2	1:D:279:TRP:CH2	2.27	0.69
1:B:302:ASN:ND2	1:C:238:ASP:HB3	2.07	0.69
2:G:175:PHE:CD2	3:K:178:SER:HB3	2.27	0.69
1:B:224:SER:HB2	1:B:279:TRP:CH2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:GLU:OE2	1:E:90:THR:HG21	1.93	0.69
1:E:224:SER:HB2	1:E:279:TRP:CH2	2.28	0.68
1:A:57:GLU:OE2	1:A:90:THR:HG21	1.94	0.68
1:C:224:SER:HB2	1:C:279:TRP:CH2	2.29	0.68
1:A:224:SER:HB2	1:A:279:TRP:CH2	2.28	0.68
1:A:226:MET:HE1	1:E:253:LEU:HD11	1.76	0.67
1:A:226:MET:HG3	4:A:349:IVM:H11A	1.74	0.67
1:D:226:MET:HG3	4:D:349:IVM:H11A	1.77	0.67
2:G:208:HIS:CE1	2:G:210:ALA:HB3	2.29	0.67
1:B:57:GLU:OE2	1:B:90:THR:HG21	1.94	0.67
1:B:317:LEU:HD21	5:B:350:LMT:O5B	1.94	0.67
1:B:250:VAL:CG1	1:C:251:THR:HG21	2.23	0.67
1:C:57:GLU:OE2	1:C:90:THR:HG21	1.94	0.67
1:B:302:ASN:HD22	1:C:238:ASP:HB3	1.60	0.67
1:E:195:THR:HA	2:J:55:ASN:HD21	1.58	0.67
1:D:253:LEU:HD11	1:E:226:MET:HE1	1.77	0.67
1:D:79:LEU:HD22	1:D:85:ILE:HD12	1.77	0.66
3:M:105:LYS:HD2	3:M:146:VAL:HG22	1.77	0.66
1:E:79:LEU:HD22	1:E:85:ILE:HD12	1.78	0.66
2:G:157:GLU:HB3	2:G:158:PRO:HA	1.77	0.66
1:D:57:GLU:OE2	1:D:90:THR:HG21	1.95	0.66
1:C:79:LEU:HD22	1:C:85:ILE:HD12	1.77	0.66
2:F:208:HIS:HD2	2:F:211:SER:H	1.44	0.66
1:A:226:MET:CE	1:E:253:LEU:HD11	2.26	0.66
1:A:234:SER:HA	1:A:237:PHE:HD2	1.61	0.65
2:J:164:ASN:CB	2:J:167:SER:HB3	2.26	0.65
3:K:132:LYS:NZ	3:K:182:THR:HG23	2.11	0.65
3:O:149:VAL:HB	3:O:164:THR:HG21	1.78	0.65
1:D:102:THR:HA	1:D:106:PRO:HA	1.78	0.65
3:L:135:LEU:HB2	3:L:181:LEU:HB3	1.77	0.65
1:A:210:LYS:CE	5:A:351:LMT:O3B	2.44	0.65
1:E:226:MET:HB2	4:E:349:IVM:H4B	1.79	0.65
1:E:234:SER:HA	1:E:237:PHE:HD2	1.61	0.65
1:B:234:SER:HA	1:B:237:PHE:HD2	1.61	0.65
1:E:102:THR:HA	1:E:106:PRO:HA	1.79	0.64
3:M:39:GLN:HB2	3:M:49:LEU:HD21	1.79	0.64
1:C:234:SER:HA	1:C:237:PHE:HD2	1.62	0.64
1:B:102:THR:HA	1:B:106:PRO:HA	1.79	0.64
1:A:102:THR:HA	1:A:106:PRO:HA	1.79	0.64
1:D:253:LEU:HD11	1:E:226:MET:CE	2.27	0.64
3:N:39:GLN:HB2	3:N:49:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:107:THR:HG21	3:O:144:PRO:HB3	1.78	0.64
3:L:39:GLN:HB2	3:L:49:LEU:HD21	1.80	0.64
1:D:234:SER:HA	1:D:237:PHE:HD2	1.61	0.64
3:O:169:LYS:HA	3:O:175:TYR:HA	1.79	0.64
1:A:79:LEU:HD22	1:A:85:ILE:HD12	1.80	0.63
1:C:102:THR:HA	1:C:106:PRO:HA	1.79	0.63
1:B:79:LEU:HD22	1:B:85:ILE:HD12	1.79	0.63
3:O:39:GLN:HB2	3:O:49:LEU:HD21	1.80	0.63
1:D:194:VAL:HG13	2:I:52:ASN:HD22	1.64	0.62
3:K:39:GLN:HB2	3:K:49:LEU:HD21	1.80	0.62
3:O:118:VAL:O	3:O:207:LYS:HE3	1.99	0.62
2:F:208:HIS:CD2	2:F:211:SER:H	2.18	0.62
2:H:128:PRO:HD3	2:H:208:HIS:ND1	2.14	0.61
1:A:42:ILE:HD13	1:A:209:LEU:HD13	1.82	0.61
1:B:73:GLN:HB3	1:B:74:PRO:HD2	1.82	0.61
2:J:179:LEU:HD13	2:J:184:TYR:CE1	2.35	0.61
3:K:170:GLN:HG2	3:K:174:LYS:O	2.00	0.61
1:E:42:ILE:HD13	1:E:209:LEU:HD13	1.82	0.61
1:E:247:THR:HG1	10:E:351:RI5:H13	1.64	0.61
2:H:50:LEU:HD21	2:H:59:SER:HB3	1.82	0.61
2:I:147:LEU:HD12	2:I:202:VAL:HG11	1.83	0.61
2:G:50:LEU:HD21	2:G:59:SER:HB3	1.83	0.61
2:I:50:LEU:HD21	2:I:59:SER:HB3	1.82	0.61
1:E:85:ILE:HD11	1:E:112:ILE:HD11	1.83	0.61
1:B:85:ILE:HD11	1:B:112:ILE:HD11	1.83	0.61
1:B:194:VAL:HG13	2:F:52:ASN:HD22	1.65	0.61
1:C:73:GLN:HB3	1:C:74:PRO:HD2	1.81	0.61
1:C:19:ARG:HH11	1:C:157:ASP:HA	1.67	0.60
3:N:159:THR:HG23	3:N:160:GLN:HG2	1.82	0.60
1:B:42:ILE:HD13	1:B:209:LEU:HD13	1.83	0.60
2:F:50:LEU:HD21	2:F:59:SER:HB3	1.83	0.60
1:E:73:GLN:HB3	1:E:74:PRO:HD2	1.83	0.60
5:A:350:LMT:C6'	5:A:350:LMT:H1B	2.32	0.60
1:D:19:ARG:HH11	1:D:157:ASP:HA	1.65	0.60
2:J:50:LEU:HD21	2:J:59:SER:HB3	1.83	0.60
1:A:19:ARG:HH11	1:A:157:ASP:HA	1.67	0.60
1:A:303:ALA:HB2	5:A:350:LMT:H6D	1.84	0.60
1:D:85:ILE:HD11	1:D:112:ILE:HD11	1.82	0.60
1:A:73:GLN:HB3	1:A:74:PRO:HD2	1.82	0.60
1:A:88:PRO:HB3	1:A:158:ILE:HD11	1.84	0.60
1:B:19:ARG:HH11	1:B:157:ASP:HA	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HD11	1:A:112:ILE:HD11	1.84	0.60
1:B:88:PRO:HB3	1:B:158:ILE:HD11	1.84	0.60
1:D:73:GLN:HB3	1:D:74:PRO:HD2	1.82	0.60
1:E:19:ARG:HH11	1:E:157:ASP:HA	1.67	0.60
1:A:299:HIS:NE2	5:A:350:LMT:H11	2.18	0.59
1:C:42:ILE:HD13	1:C:209:LEU:HD13	1.83	0.59
1:C:85:ILE:HD11	1:C:112:ILE:HD11	1.84	0.59
1:D:42:ILE:HD13	1:D:209:LEU:HD13	1.84	0.59
3:K:132:LYS:HZ1	3:K:182:THR:HG23	1.67	0.59
3:L:41:LYS:HE2	3:L:83:GLU:O	2.02	0.59
1:B:17:ARG:HB3	1:C:80:THR:HB	1.84	0.59
1:E:88:PRO:HB3	1:E:158:ILE:HD11	1.85	0.59
1:C:88:PRO:HB3	1:C:158:ILE:HD11	1.85	0.58
1:D:88:PRO:HB3	1:D:158:ILE:HD11	1.85	0.58
1:E:226:MET:HG3	4:E:349:IVM:H11A	1.85	0.58
1:B:236:TRP:HH2	5:B:350:LMT:H12	1.68	0.58
3:O:41:LYS:HE2	3:O:83:GLU:O	2.02	0.58
1:A:195:THR:HA	2:H:55:ASN:HD21	1.68	0.58
3:M:41:LYS:HE2	3:M:83:GLU:O	2.03	0.58
3:N:41:LYS:HE2	3:N:83:GLU:O	2.03	0.58
1:B:232:TRP:CH2	1:B:324:PRO:HA	2.39	0.58
3:M:122:PRO:HG3	3:M:209:LEU:HD11	1.85	0.58
1:E:232:TRP:CH2	1:E:324:PRO:HA	2.38	0.58
1:C:232:TRP:CH2	1:C:324:PRO:HA	2.39	0.58
2:H:50:LEU:CD2	2:H:59:SER:HB3	2.34	0.57
3:M:154:ASP:HA	3:M:193:SER:HB3	1.85	0.57
3:K:41:LYS:HE2	3:K:83:GLU:O	2.04	0.57
2:G:50:LEU:CD2	2:G:59:SER:HB3	2.34	0.57
2:I:50:LEU:CD2	2:I:59:SER:HB3	2.34	0.57
2:J:50:LEU:CD2	2:J:59:SER:HB3	2.34	0.57
3:O:151:TRP:CD2	3:O:181:LEU:HD12	2.40	0.57
1:B:224:SER:HB2	1:B:279:TRP:HH2	1.70	0.57
1:A:232:TRP:CH2	1:A:324:PRO:HA	2.38	0.57
1:D:36:LEU:HD23	1:D:39:ILE:HD11	1.87	0.56
1:D:232:TRP:CH2	1:D:324:PRO:HA	2.40	0.56
2:F:50:LEU:CD2	2:F:59:SER:HB3	2.34	0.56
2:J:162:THR:OG1	2:J:205:ASN:HB2	2.04	0.56
1:D:224:SER:HB2	1:D:279:TRP:HH2	1.69	0.56
1:E:285:THR:HG21	7:E:350:OCT:H21	1.85	0.56
1:D:250:VAL:CG1	1:E:251:THR:HG21	2.36	0.56
2:H:179:LEU:HD13	2:H:184:TYR:CE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LEU:HD11	1:D:226:MET:CE	2.36	0.56
1:E:36:LEU:HD23	1:E:39:ILE:HD11	1.88	0.56
1:A:239:ARG:CZ	1:A:313:LYS:HG2	2.36	0.56
1:C:253:LEU:HD11	1:D:226:MET:HE1	1.88	0.56
1:A:36:LEU:HD23	1:A:39:ILE:HD11	1.88	0.56
3:K:22:CYS:O	3:K:72:LYS:HB2	2.06	0.56
1:A:39:ILE:HD13	1:A:207:ILE:CD1	2.36	0.56
1:B:36:LEU:HD23	1:B:39:ILE:HD11	1.87	0.55
1:C:239:ARG:CZ	1:C:313:LYS:HG2	2.36	0.55
1:D:226:MET:HB2	4:D:349:IVM:H4B	1.87	0.55
1:A:66:TYR:CE2	1:A:114:ASN:HA	2.41	0.55
1:E:239:ARG:CZ	1:E:313:LYS:HG2	2.36	0.55
1:A:224:SER:HB2	1:A:279:TRP:HH2	1.70	0.55
1:B:39:ILE:HD13	1:B:207:ILE:CD1	2.36	0.55
1:C:39:ILE:HD13	1:C:207:ILE:CD1	2.36	0.55
1:C:66:TYR:CE2	1:C:114:ASN:HA	2.42	0.55
1:B:66:TYR:CE2	1:B:114:ASN:HA	2.42	0.55
1:E:66:TYR:CE2	1:E:114:ASN:HA	2.41	0.55
2:G:133:LEU:HB2	2:G:148:GLY:O	2.06	0.55
2:H:157:GLU:HG3	2:H:184:TYR:CD2	2.41	0.55
3:L:206:GLU:O	3:L:207:LYS:HD2	2.05	0.55
3:M:22:CYS:O	3:M:72:LYS:HB2	2.06	0.55
3:M:37:TRP:CE2	3:M:75:LEU:HB2	2.42	0.55
3:L:37:TRP:CE2	3:L:75:LEU:HB2	2.40	0.55
1:B:273:ILE:HD11	4:C:350:IVM:H30	1.87	0.55
2:H:186:LEU:HD12	2:H:186:LEU:C	2.27	0.55
2:J:101:ASP:HB3	2:J:104:ARG:HG3	1.89	0.55
3:N:37:TRP:CE2	3:N:75:LEU:HB2	2.41	0.55
1:B:239:ARG:CZ	1:B:313:LYS:HG2	2.37	0.55
2:J:203:THR:HA	2:J:218:LYS:HA	1.88	0.55
3:O:37:TRP:CE2	3:O:75:LEU:HB2	2.42	0.55
1:B:226:MET:HG3	4:B:349:IVM:H11A	1.89	0.55
1:D:17:ARG:HB3	1:E:80:THR:HB	1.89	0.55
1:D:224:SER:HB2	1:D:279:TRP:CZ3	2.42	0.55
1:D:239:ARG:CZ	1:D:313:LYS:HG2	2.37	0.55
1:E:224:SER:HB2	1:E:279:TRP:CZ3	2.42	0.55
3:L:107:THR:HG21	3:L:144:PRO:CB	2.28	0.55
1:C:224:SER:HB2	1:C:279:TRP:HH2	1.70	0.54
1:B:224:SER:HB2	1:B:279:TRP:CZ3	2.42	0.54
1:D:66:TYR:CE2	1:D:114:ASN:HA	2.41	0.54
1:E:39:ILE:HD13	1:E:207:ILE:CD1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:HD23	1:C:39:ILE:HD11	1.88	0.54
2:G:155:PHE:CD2	2:G:156:PRO:HA	2.43	0.54
2:H:101:ASP:HB3	2:H:104:ARG:HG3	1.90	0.54
3:N:170:GLN:O	3:N:171:SER:C	2.46	0.54
1:D:234:SER:HG	1:D:294:PHE:HZ	1.54	0.54
1:D:242:ILE:N	1:D:243:PRO:CD	2.70	0.54
1:D:260:SER:HG	4:E:349:IVM:HO10	1.56	0.54
2:F:101:ASP:HB3	2:F:104:ARG:HG3	1.89	0.54
3:M:111:GLN:HB2	3:M:112:PRO:HD2	1.87	0.54
3:O:22:CYS:O	3:O:72:LYS:HB2	2.07	0.54
5:A:350:LMT:H1B	5:A:350:LMT:H6E	1.90	0.54
1:C:234:SER:HG	1:C:294:PHE:HZ	1.56	0.54
1:E:230:VAL:O	1:E:233:VAL:HG22	2.07	0.54
1:E:242:ILE:N	1:E:243:PRO:CD	2.71	0.54
2:G:101:ASP:HB3	2:G:104:ARG:HG3	1.89	0.54
3:N:22:CYS:O	3:N:72:LYS:HB2	2.07	0.54
1:A:224:SER:HB2	1:A:279:TRP:CZ3	2.43	0.54
1:B:242:ILE:N	1:B:243:PRO:CD	2.71	0.54
1:A:210:LYS:NZ	5:A:351:LMT:O3B	2.40	0.54
1:A:234:SER:HA	1:A:237:PHE:CD2	2.43	0.54
1:E:222:ILE:HG23	4:E:349:IVM:H2A	1.90	0.54
2:I:101:ASP:HB3	2:I:104:ARG:HG3	1.89	0.54
3:L:22:CYS:O	3:L:72:LYS:HB2	2.08	0.54
1:A:230:VAL:O	1:A:233:VAL:HG22	2.08	0.53
1:A:250:VAL:CG1	1:B:251:THR:HG21	2.38	0.53
2:H:6:GLN:H	2:H:114:GLN:HE22	1.56	0.53
3:M:9:ALA:HB2	3:M:146:VAL:HG21	1.90	0.53
1:B:230:VAL:O	1:B:233:VAL:HG22	2.08	0.53
1:D:230:VAL:O	1:D:233:VAL:HG22	2.08	0.53
2:G:6:GLN:H	2:G:114:GLN:HE22	1.56	0.53
1:C:230:VAL:O	1:C:233:VAL:HG22	2.08	0.53
1:D:39:ILE:HD13	1:D:207:ILE:CD1	2.37	0.53
3:K:37:TRP:CE2	3:K:75:LEU:HB2	2.42	0.53
3:N:169:LYS:NZ	3:N:169:LYS:HB3	2.24	0.53
1:A:234:SER:HG	1:A:294:PHE:HZ	1.55	0.53
1:C:242:ILE:N	1:C:243:PRO:CD	2.71	0.53
1:A:84:GLN:HE21	1:A:84:GLN:HA	1.74	0.53
1:D:242:ILE:HG22	1:D:243:PRO:HD3	1.91	0.53
2:I:171:GLY:O	2:I:190:VAL:HA	2.08	0.53
1:A:242:ILE:N	1:A:243:PRO:CD	2.71	0.53
1:B:189:THR:HG22	1:B:190:TYR:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:163:TRP:HZ2	2:H:188:SER:O	1.91	0.53
2:I:131:TYR:CE1	3:O:126:GLU:HB3	2.44	0.53
1:C:224:SER:HB2	1:C:279:TRP:CZ3	2.44	0.53
1:D:189:THR:HG22	1:D:190:TYR:H	1.73	0.53
3:O:164:THR:HG22	3:O:179:SER:OG	2.09	0.53
1:D:195:THR:HA	2:I:55:ASN:HD22	1.73	0.52
2:G:110:ASP:HB3	2:G:111:TYR:CD2	2.44	0.52
2:J:110:ASP:HB3	2:J:111:TYR:CD2	2.44	0.52
1:A:189:THR:HG22	1:A:190:TYR:H	1.74	0.52
1:D:19:ARG:HG2	1:D:20:PRO:HD2	1.92	0.52
2:G:157:GLU:HG3	2:G:184:TYR:CD2	2.43	0.52
1:C:234:SER:HA	1:C:237:PHE:CD2	2.44	0.52
2:I:203:THR:HG22	2:I:218:LYS:HA	1.92	0.52
3:O:42:PRO:O	3:O:43:ASP:HB2	2.09	0.52
1:E:154:THR:HG23	1:E:156:LYS:H	1.74	0.52
1:E:234:SER:HG	1:E:294:PHE:HZ	1.57	0.52
2:H:110:ASP:HB3	2:H:111:TYR:CD2	2.44	0.52
1:A:19:ARG:HG2	1:A:20:PRO:HD2	1.90	0.52
1:B:242:ILE:HG22	1:B:243:PRO:HD3	1.92	0.52
1:C:154:THR:HG23	1:C:156:LYS:H	1.75	0.52
2:F:110:ASP:HB3	2:F:111:TYR:CD2	2.45	0.52
2:F:164:ASN:HB2	2:F:167:SER:HB2	1.91	0.52
3:N:42:PRO:O	3:N:43:ASP:HB2	2.10	0.52
1:A:242:ILE:HG22	1:A:243:PRO:HD3	1.92	0.52
1:E:224:SER:HB2	1:E:279:TRP:HH2	1.69	0.52
1:B:84:GLN:HA	1:B:84:GLN:HE21	1.75	0.52
1:C:220:LEU:HD11	1:C:280:ILE:HD11	1.92	0.52
10:E:351:RI5:C03	10:E:351:RI5:O20	2.58	0.52
1:B:154:THR:HG23	1:B:156:LYS:H	1.75	0.52
1:C:195:THR:HA	2:G:55:ASN:HD21	1.74	0.52
1:E:242:ILE:HG22	1:E:243:PRO:HD3	1.91	0.52
3:M:147:VAL:HG12	3:M:200:HIS:HB2	1.90	0.52
3:O:111:GLN:HG2	3:O:112:PRO:HD2	1.92	0.52
1:E:84:GLN:HE21	1:E:84:GLN:HA	1.75	0.51
1:E:189:THR:HG22	1:E:190:TYR:H	1.75	0.51
3:M:42:PRO:O	3:M:43:ASP:HB2	2.10	0.51
1:B:234:SER:HA	1:B:237:PHE:CD2	2.43	0.51
3:O:170:GLN:OE1	3:O:176:MET:HB3	2.10	0.51
2:J:6:GLN:H	2:J:114:GLN:HE22	1.59	0.51
3:O:111:GLN:HE22	3:O:174:LYS:HE3	1.75	0.51
4:A:349:IVM:H30	1:E:273:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LEU:HD12	1:C:251:THR:HG23	1.92	0.51
1:C:84:GLN:HA	1:C:84:GLN:HE21	1.76	0.51
2:F:163:TRP:CZ3	2:F:204:CYS:HB3	2.46	0.51
2:I:20:ILE:HD11	2:I:81:MET:HE1	1.93	0.51
1:A:251:THR:HG21	1:E:250:VAL:CG1	2.40	0.51
2:I:131:TYR:CD2	3:O:127:GLU:HG2	2.46	0.51
3:M:10:LEU:HD12	3:M:20:LEU:HD23	1.93	0.51
3:M:152:LYS:HG2	3:M:157:PRO:HA	1.93	0.51
3:N:10:LEU:HD12	3:N:20:LEU:HD23	1.93	0.51
2:G:148:GLY:HA2	2:G:188:SER:O	2.11	0.51
2:H:84:LEU:N	2:H:84:LEU:HD12	2.26	0.51
1:A:220:LEU:HD11	1:A:280:ILE:HD11	1.92	0.51
3:L:10:LEU:HD12	3:L:20:LEU:HD23	1.93	0.51
1:C:242:ILE:HG22	1:C:243:PRO:HD3	1.91	0.51
1:D:234:SER:HA	1:D:237:PHE:CD2	2.44	0.51
1:A:284:MET:HG3	1:B:226:MET:HE3	1.93	0.51
1:C:189:THR:HG22	1:C:190:TYR:H	1.76	0.51
2:F:84:LEU:N	2:F:84:LEU:HD12	2.26	0.51
2:G:155:PHE:CG	2:G:156:PRO:HA	2.46	0.51
3:K:10:LEU:HD12	3:K:20:LEU:HD23	1.93	0.51
3:K:42:PRO:O	3:K:43:ASP:HB2	2.10	0.51
1:C:19:ARG:HG2	1:C:20:PRO:HD2	1.92	0.50
1:E:220:LEU:HD11	1:E:280:ILE:HD11	1.93	0.50
1:A:79:LEU:HD13	1:A:112:ILE:HD11	1.93	0.50
1:B:236:TRP:CZ3	5:B:350:LMT:H12	2.46	0.50
1:C:79:LEU:HD13	1:C:112:ILE:HD11	1.93	0.50
1:D:154:THR:HG23	1:D:156:LYS:H	1.76	0.50
2:I:110:ASP:HB3	2:I:111:TYR:CD2	2.45	0.50
3:L:42:PRO:O	3:L:43:ASP:HB2	2.10	0.50
3:O:131:ASN:OD1	3:O:185:ALA:HB3	2.11	0.50
1:B:19:ARG:HG2	1:B:20:PRO:HD2	1.92	0.50
1:B:128:LEU:HD13	1:B:146:ILE:HG12	1.93	0.50
2:G:84:LEU:HD12	2:G:84:LEU:N	2.26	0.50
2:G:213:THR:HG22	2:G:215:VAL:HG23	1.93	0.50
2:J:179:LEU:HD13	2:J:184:TYR:CZ	2.47	0.50
1:A:80:THR:HB	1:E:17:ARG:HB3	1.92	0.50
1:A:302:ASN:HD22	1:B:238:ASP:HB3	1.77	0.50
1:E:19:ARG:HG2	1:E:20:PRO:HD2	1.94	0.50
2:J:220:VAL:HG23	2:J:221:PRO:HD2	1.93	0.50
3:M:105:LYS:HD2	3:M:146:VAL:CG2	2.40	0.50
1:D:286:PHE:CZ	7:D:350:OCT:H12	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:GLN:H	2:F:114:GLN:HE22	1.58	0.50
2:J:157:GLU:HB3	2:J:158:PRO:HA	1.94	0.50
1:E:234:SER:HA	1:E:237:PHE:CD2	2.43	0.50
2:I:84:LEU:N	2:I:84:LEU:HD12	2.27	0.50
2:I:100:GLY:HA3	2:I:108:TYR:CZ	2.47	0.50
2:J:84:LEU:HD12	2:J:84:LEU:N	2.26	0.50
2:F:128:PRO:HB3	2:F:154:TYR:HB3	1.93	0.50
2:H:156:PRO:HD2	2:H:210:ALA:CB	2.41	0.50
1:B:220:LEU:HD11	1:B:280:ILE:HD11	1.94	0.50
1:C:222:ILE:HG23	4:C:350:IVM:H2A	1.93	0.50
1:D:84:GLN:HE21	1:D:84:GLN:HA	1.75	0.50
1:D:260:SER:OG	4:E:349:IVM:O10	2.25	0.50
2:G:186:LEU:C	2:G:186:LEU:HD12	2.32	0.50
2:H:157:GLU:HB3	2:H:158:PRO:HA	1.93	0.50
2:G:175:PHE:CZ	3:K:138:THR:HB	2.47	0.49
2:I:6:GLN:H	2:I:114:GLN:HE22	1.58	0.49
1:D:128:LEU:HD13	1:D:146:ILE:HG12	1.93	0.49
1:E:128:LEU:HD13	1:E:146:ILE:HG12	1.93	0.49
1:D:220:LEU:HD11	1:D:280:ILE:HD11	1.93	0.49
3:O:10:LEU:HD12	3:O:20:LEU:HD23	1.94	0.49
1:D:126:LEU:HD13	1:D:128:LEU:HD21	1.95	0.49
1:D:254:LEU:HD12	1:E:251:THR:HG23	1.95	0.49
1:E:79:LEU:HD13	1:E:112:ILE:HD11	1.95	0.49
1:A:154:THR:HG23	1:A:156:LYS:H	1.76	0.49
1:B:126:LEU:HD13	1:B:128:LEU:HD21	1.95	0.49
1:D:243:PRO:HB3	10:E:351:RI5:C03	2.42	0.49
2:G:133:LEU:HD11	3:K:136:VAL:HG21	1.95	0.49
2:F:100:GLY:HA3	2:F:108:TYR:CZ	2.47	0.49
2:G:175:PHE:HZ	3:K:138:THR:HB	1.77	0.49
1:A:137:TYR:HB3	1:A:138:PRO:HD3	1.93	0.49
2:G:100:GLY:HA3	2:G:108:TYR:CZ	2.48	0.49
2:H:100:GLY:HA3	2:H:108:TYR:CZ	2.48	0.49
1:B:137:TYR:HB3	1:B:138:PRO:HD3	1.94	0.49
1:E:70:GLY:C	1:E:72:GLY:H	2.16	0.49
1:E:137:TYR:HB3	1:E:138:PRO:HD3	1.93	0.49
1:A:302:ASN:ND2	1:B:238:ASP:HB3	2.27	0.49
2:H:147:LEU:HD12	2:H:202:VAL:HG21	1.93	0.49
1:A:70:GLY:C	1:A:72:GLY:H	2.16	0.49
1:C:17:ARG:HB3	1:D:80:THR:CB	2.42	0.49
2:H:2:VAL:HG21	2:H:111:TYR:CD2	2.48	0.49
2:H:34:MET:CE	2:H:96:CYS:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:34:MET:CE	2:I:96:CYS:HB2	2.43	0.48
2:J:100:GLY:HA3	2:J:108:TYR:CZ	2.48	0.48
3:K:125:SER:HA	3:K:128:LEU:HD12	1.95	0.48
1:C:128:LEU:HD13	1:C:146:ILE:HG12	1.93	0.48
2:H:100:GLY:HA3	2:H:108:TYR:CE1	2.48	0.48
2:J:34:MET:CE	2:J:96:CYS:HB2	2.43	0.48
2:J:175:PHE:HD1	2:J:187:SER:O	1.96	0.48
1:B:284:MET:HG3	1:C:226:MET:HE3	1.96	0.48
1:C:70:GLY:C	1:C:72:GLY:H	2.15	0.48
1:D:79:LEU:HD13	1:D:112:ILE:HD11	1.96	0.48
2:G:100:GLY:HA3	2:G:108:TYR:CE1	2.48	0.48
1:C:137:TYR:HB3	1:C:138:PRO:HD3	1.94	0.48
1:D:137:TYR:HB3	1:D:138:PRO:HD3	1.95	0.48
2:J:100:GLY:HA3	2:J:108:TYR:CE1	2.48	0.48
1:C:126:LEU:HD13	1:C:128:LEU:HD21	1.96	0.48
1:E:286:PHE:CE2	7:E:350:OCT:H12	2.49	0.48
3:K:120:LEU:HD12	3:K:196:CYS:HB3	1.94	0.48
3:M:123:PRO:HD2	3:M:188:TRP:CH2	2.49	0.48
1:B:70:GLY:C	1:B:72:GLY:H	2.16	0.48
2:F:34:MET:CE	2:F:96:CYS:HB2	2.43	0.48
2:I:100:GLY:HA3	2:I:108:TYR:CE1	2.49	0.48
1:B:243:PRO:HB3	10:E:351:RI5:H05	1.95	0.48
2:F:100:GLY:HA3	2:F:108:TYR:CE1	2.49	0.48
1:A:128:LEU:HD13	1:A:146:ILE:HG12	1.95	0.48
1:C:222:ILE:N	1:C:223:PRO:HD2	2.29	0.48
1:E:96:LYS:HD2	1:E:129:SER:HB3	1.96	0.48
2:H:128:PRO:HB3	2:H:154:TYR:HB3	1.96	0.48
1:D:70:GLY:C	1:D:72:GLY:H	2.17	0.47
2:J:2:VAL:HG21	2:J:111:TYR:CD2	2.49	0.47
1:A:242:ILE:HD11	1:A:294:PHE:HB3	1.97	0.47
1:E:242:ILE:HD11	1:E:294:PHE:HB3	1.96	0.47
1:E:243:PRO:HB2	10:E:351:RI5:C03	2.44	0.47
2:G:2:VAL:HG21	2:G:111:TYR:CD2	2.49	0.47
3:M:11:THR:HG23	3:M:109:LEU:HD13	1.96	0.47
2:F:177:ALA:HB2	2:F:186:LEU:HD23	1.96	0.47
1:B:96:LYS:HD2	1:B:129:SER:HB3	1.96	0.47
2:I:2:VAL:HG21	2:I:111:TYR:CD2	2.49	0.47
3:K:107:THR:HG21	3:K:144:PRO:HB3	1.95	0.47
3:N:164:THR:HA	3:N:179:SER:HA	1.96	0.47
1:A:130:CYS:O	1:A:132:MET:HG3	2.15	0.47
1:A:303:ALA:CB	5:A:350:LMT:H6D	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:VAL:HG21	2:F:111:TYR:CD2	2.49	0.47
1:A:222:ILE:N	1:A:223:PRO:HD2	2.30	0.47
2:G:34:MET:CE	2:G:96:CYS:HB2	2.45	0.47
2:J:30:THR:HA	2:J:53:PRO:HB2	1.97	0.47
2:J:128:PRO:HD3	2:J:208:HIS:ND1	2.30	0.47
1:B:195:THR:HA	2:F:55:ASN:HD22	1.76	0.47
1:B:224:SER:CB	1:B:279:TRP:CZ3	2.98	0.47
2:H:179:LEU:HD13	2:H:184:TYR:CD1	2.50	0.47
1:E:126:LEU:HD13	1:E:128:LEU:HD21	1.96	0.47
3:L:120:LEU:HD23	3:L:120:LEU:C	2.35	0.47
1:B:187:SER:HB3	6:B:400:NAG:O7	2.15	0.47
1:D:222:ILE:N	1:D:223:PRO:HD2	2.30	0.47
1:D:224:SER:CB	1:D:279:TRP:CZ3	2.97	0.47
1:B:53:LEU:H	1:B:53:LEU:HD23	1.80	0.46
1:B:79:LEU:HD13	1:B:112:ILE:HD11	1.96	0.46
3:M:50:ILE:HG22	3:M:51:GLY:N	2.30	0.46
3:N:41:LYS:HB2	3:N:45:LEU:HB2	1.97	0.46
1:B:128:LEU:CD1	1:B:146:ILE:HG12	2.45	0.46
2:I:30:THR:HA	2:I:53:PRO:HB2	1.97	0.46
1:A:227:LEU:HD21	1:A:255:THR:CG2	2.46	0.46
1:D:96:LYS:HD2	1:D:129:SER:HB3	1.98	0.46
1:D:242:ILE:HD11	1:D:294:PHE:HB3	1.96	0.46
2:I:131:TYR:CD1	3:O:126:GLU:HB3	2.50	0.46
3:K:41:LYS:HB2	3:K:45:LEU:HB2	1.97	0.46
1:A:126:LEU:HD13	1:A:128:LEU:HD21	1.97	0.46
1:C:96:LYS:HD2	1:C:129:SER:HB3	1.97	0.46
1:C:128:LEU:CD1	1:C:146:ILE:HG12	2.46	0.46
1:E:194:VAL:HG13	2:J:52:ASN:HD22	1.81	0.46
1:A:226:MET:O	1:A:230:VAL:HG23	2.16	0.46
1:B:222:ILE:N	1:B:223:PRO:HD2	2.31	0.46
2:G:173:HIS:HB3	3:K:176:MET:SD	2.55	0.46
3:M:10:LEU:HD12	3:M:20:LEU:CD2	2.46	0.46
3:N:142:PHE:CE1	3:N:145:GLY:HA2	2.50	0.46
3:O:41:LYS:HB2	3:O:45:LEU:HB2	1.98	0.46
1:A:103:ILE:HD12	1:A:103:ILE:HA	1.77	0.46
1:A:224:SER:CB	1:A:279:TRP:CZ3	2.99	0.46
1:D:128:LEU:CD1	1:D:146:ILE:HG12	2.46	0.46
2:G:151:VAL:HG12	2:G:154:TYR:CD1	2.51	0.46
3:M:143:TYR:HA	3:M:144:PRO:C	2.36	0.46
3:N:142:PHE:HE1	3:N:145:GLY:HA2	1.81	0.46
1:B:227:LEU:HD21	1:B:255:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:HD13	1:C:168:LEU:HD11	1.98	0.46
1:C:130:CYS:O	1:C:132:MET:HG3	2.16	0.46
1:C:226:MET:O	1:C:230:VAL:HG23	2.16	0.46
1:E:222:ILE:N	1:E:223:PRO:HD2	2.30	0.46
2:J:152:LYS:HA	2:J:185:THR:HG23	1.98	0.46
3:O:151:TRP:CE3	3:O:181:LEU:HD12	2.50	0.46
1:C:34:MET:HG3	1:C:53:LEU:HD12	1.98	0.46
1:C:242:ILE:HD11	1:C:294:PHE:HB3	1.98	0.46
1:D:53:LEU:H	1:D:53:LEU:HD23	1.80	0.46
1:D:130:CYS:O	1:D:132:MET:HG3	2.16	0.46
1:E:53:LEU:HD23	1:E:53:LEU:H	1.81	0.46
2:J:20:ILE:HD11	2:J:81:MET:HE1	1.96	0.46
3:M:50:ILE:HG22	3:M:51:GLY:H	1.80	0.46
1:B:234:SER:HG	1:B:294:PHE:HZ	1.60	0.46
1:B:242:ILE:HD11	1:B:294:PHE:HB3	1.97	0.46
1:C:224:SER:CB	1:C:279:TRP:CZ3	2.99	0.46
3:K:50:ILE:HG22	3:K:51:GLY:N	2.31	0.46
3:L:122:PRO:HB3	3:L:209:LEU:HD11	1.97	0.46
3:M:172:ASN:OD1	3:M:174:LYS:HD3	2.16	0.46
1:C:152:ALA:HB1	1:D:109:LEU:HD13	1.97	0.45
1:E:224:SER:CB	1:E:279:TRP:CZ3	2.99	0.45
2:G:30:THR:HA	2:G:53:PRO:HB2	1.97	0.45
2:G:133:LEU:HB3	3:K:121:PHE:CD1	2.51	0.45
2:H:30:THR:HA	2:H:53:PRO:HB2	1.97	0.45
3:L:10:LEU:HD12	3:L:20:LEU:CD2	2.46	0.45
1:B:130:CYS:O	1:B:132:MET:HG3	2.16	0.45
1:C:226:MET:HB2	4:C:350:IVM:H4B	1.98	0.45
1:D:103:ILE:HD12	1:D:103:ILE:HA	1.79	0.45
2:J:133:LEU:HD21	2:J:150:LEU:HB2	1.96	0.45
3:O:50:ILE:HG22	3:O:51:GLY:N	2.32	0.45
1:A:96:LYS:HD2	1:A:129:SER:HB3	1.97	0.45
2:H:197:TRP:CD1	2:H:202:VAL:HG22	2.51	0.45
1:A:20:PRO:HA	1:A:21:PRO:HD3	1.85	0.45
1:B:39:ILE:HD13	1:B:207:ILE:HD13	1.99	0.45
2:F:30:THR:HA	2:F:53:PRO:HB2	1.97	0.45
2:J:133:LEU:HB3	3:M:121:PHE:CD1	2.51	0.45
3:M:41:LYS:HD3	3:M:86:ALA:HB2	1.98	0.45
1:C:20:PRO:HA	1:C:21:PRO:HD3	1.83	0.45
1:E:194:VAL:HG13	2:J:52:ASN:HB2	1.99	0.45
2:H:107:ARG:NH1	3:L:34:PHE:CZ	2.84	0.45
2:H:164:ASN:OD1	2:H:202:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:125:THR:HG21	2:I:210:ALA:O	2.17	0.45
3:N:10:LEU:HD12	3:N:20:LEU:CD2	2.47	0.45
1:A:84:GLN:HA	1:A:84:GLN:NE2	2.32	0.45
1:A:227:LEU:HD21	1:A:255:THR:HG22	1.99	0.45
1:C:323:PHE:HB2	1:C:324:PRO:HD3	1.99	0.45
1:E:128:LEU:CD1	1:E:146:ILE:HG12	2.46	0.45
3:L:41:LYS:HB2	3:L:45:LEU:HB2	1.98	0.45
3:O:169:LYS:CG	3:O:173:ASN:HA	2.46	0.45
1:B:36:LEU:HD13	1:B:168:LEU:HD11	1.99	0.45
2:J:14:PRO:HD2	2:J:122:SER:HB3	1.99	0.45
2:J:164:ASN:HB3	2:J:167:SER:HB3	1.98	0.45
1:A:146:ILE:HB	1:A:205:THR:CG2	2.46	0.45
3:K:10:LEU:HD12	3:K:20:LEU:CD2	2.46	0.45
1:B:226:MET:O	1:B:230:VAL:HG23	2.17	0.45
1:D:227:LEU:HD21	1:D:255:THR:CG2	2.47	0.45
3:L:41:LYS:HD3	3:L:86:ALA:HB2	1.98	0.45
1:B:250:VAL:HG12	1:C:251:THR:HG21	1.97	0.45
1:E:130:CYS:O	1:E:132:MET:HG3	2.16	0.45
1:E:227:LEU:HD21	1:E:255:THR:CG2	2.47	0.45
3:K:41:LYS:HD3	3:K:86:ALA:HB2	1.99	0.45
3:O:50:ILE:HG22	3:O:51:GLY:H	1.82	0.45
1:A:128:LEU:CD1	1:A:146:ILE:HG12	2.47	0.44
1:A:254:LEU:HD12	1:B:251:THR:HG23	1.98	0.44
1:B:227:LEU:HD21	1:B:255:THR:HG22	1.99	0.44
1:E:36:LEU:HD13	1:E:168:LEU:HD11	1.98	0.44
1:E:323:PHE:HB2	1:E:324:PRO:HD3	1.99	0.44
2:I:36:TRP:CD1	2:I:70:LEU:HD22	2.52	0.44
1:B:323:PHE:HB2	1:B:324:PRO:HD3	1.99	0.44
1:C:42:ILE:HD12	1:C:181:PHE:CD2	2.53	0.44
1:D:84:GLN:HA	1:D:84:GLN:NE2	2.33	0.44
1:E:195:THR:HA	2:J:55:ASN:HD22	1.77	0.44
3:M:41:LYS:HB2	3:M:45:LEU:HB2	1.98	0.44
3:M:209:LEU:HD23	3:M:210:SER:N	2.32	0.44
1:A:163:LYS:O	1:A:167:PRO:HG3	2.17	0.44
1:B:146:ILE:HB	1:B:205:THR:CG2	2.48	0.44
3:K:50:ILE:HG22	3:K:51:GLY:H	1.82	0.44
3:M:153:VAL:HG22	3:M:194:TYR:CD2	2.52	0.44
1:A:39:ILE:HD13	1:A:207:ILE:HD13	1.99	0.44
2:J:33:THR:HA	2:J:53:PRO:HD3	2.00	0.44
3:N:41:LYS:HD3	3:N:86:ALA:HB2	1.99	0.44
3:O:41:LYS:HD3	3:O:86:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HD13	1:A:168:LEU:HD11	1.99	0.44
1:A:303:ALA:HB1	5:A:350:LMT:O2B	2.18	0.44
1:B:84:GLN:HA	1:B:84:GLN:NE2	2.32	0.44
1:B:317:LEU:HG	5:B:350:LMT:H6E	2.00	0.44
1:C:67:GLY:O	1:C:70:GLY:N	2.49	0.44
1:E:84:GLN:HA	1:E:84:GLN:NE2	2.33	0.44
1:E:146:ILE:HB	1:E:205:THR:CG2	2.48	0.44
1:E:163:LYS:O	1:E:167:PRO:HG3	2.17	0.44
1:E:226:MET:O	1:E:230:VAL:HG23	2.17	0.44
1:A:53:LEU:HD23	1:A:53:LEU:H	1.82	0.44
1:D:302:ASN:ND2	1:E:238:ASP:HB3	2.33	0.44
1:E:243:PRO:CG	10:E:351:RI5:H03	2.46	0.44
2:G:33:THR:HA	2:G:53:PRO:HD3	2.00	0.44
3:L:50:ILE:HG22	3:L:51:GLY:H	1.83	0.44
3:L:50:ILE:HG22	3:L:51:GLY:N	2.32	0.44
1:A:138:PRO:HB2	1:A:139:MET:SD	2.58	0.44
1:B:138:PRO:HB2	1:B:139:MET:SD	2.58	0.44
1:C:39:ILE:HD13	1:C:207:ILE:HD13	2.00	0.44
1:C:243:PRO:HB3	10:E:351:RI5:H04	2.00	0.44
2:I:131:TYR:CE2	3:O:127:GLU:HG2	2.53	0.44
3:O:10:LEU:HD12	3:O:20:LEU:CD2	2.47	0.44
1:A:17:ARG:HB3	1:B:80:THR:HB	2.00	0.44
1:E:90:THR:HG22	1:E:160:TYR:HH	1.80	0.44
2:H:180:GLN:O	2:H:181:SER:HB2	2.18	0.44
1:D:226:MET:O	1:D:230:VAL:HG23	2.17	0.44
2:H:33:THR:HA	2:H:53:PRO:HD3	2.00	0.44
1:B:42:ILE:HD12	1:B:181:PHE:CD2	2.53	0.43
1:D:163:LYS:O	1:D:167:PRO:HG3	2.18	0.43
1:E:141:VAL:HG12	1:E:210:LYS:HA	2.00	0.43
2:F:33:THR:HA	2:F:53:PRO:HD3	1.99	0.43
2:I:33:THR:HA	2:I:53:PRO:HD3	2.00	0.43
2:I:131:TYR:HD1	3:O:126:GLU:OE1	2.01	0.43
1:C:227:LEU:HD21	1:C:255:THR:CG2	2.48	0.43
1:D:42:ILE:HD12	1:D:181:PHE:CD2	2.53	0.43
1:D:141:VAL:HG12	1:D:210:LYS:HA	1.99	0.43
3:L:108:VAL:O	3:L:143:TYR:OH	2.37	0.43
3:N:50:ILE:HG22	3:N:51:GLY:N	2.32	0.43
1:A:323:PHE:HB2	1:A:324:PRO:HD3	1.99	0.43
1:C:146:ILE:HB	1:C:205:THR:CG2	2.48	0.43
1:D:34:MET:HG3	1:D:53:LEU:HD12	2.01	0.43
1:D:146:ILE:HB	1:D:205:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ILE:HD12	1:E:181:PHE:CD2	2.53	0.43
2:G:162:THR:OG1	2:G:205:ASN:HB2	2.18	0.43
2:H:128:PRO:CA	2:H:154:TYR:HB3	2.48	0.43
2:I:198:PRO:HG3	2:I:221:PRO:HG3	2.00	0.43
2:J:200:GLU:O	2:J:202:VAL:HG23	2.18	0.43
3:M:166:GLN:HG3	3:M:167:PRO:HD2	1.98	0.43
3:N:50:ILE:HG22	3:N:51:GLY:H	1.83	0.43
1:A:210:LYS:HE2	5:A:351:LMT:O3B	2.16	0.43
1:B:163:LYS:O	1:B:167:PRO:HG3	2.19	0.43
1:E:138:PRO:HB2	1:E:139:MET:SD	2.59	0.43
2:H:154:TYR:O	2:H:155:PHE:HB2	2.19	0.43
3:N:41:LYS:HB3	3:N:42:PRO:HD2	2.01	0.43
1:A:34:MET:HG3	1:A:53:LEU:HD12	2.00	0.43
1:B:103:ILE:HD12	1:B:103:ILE:HA	1.78	0.43
1:D:20:PRO:HA	1:D:21:PRO:HD3	1.83	0.43
1:E:39:ILE:HD13	1:E:207:ILE:HD13	2.00	0.43
2:F:131:TYR:HB3	3:N:124:SER:OG	2.18	0.43
1:D:323:PHE:HB2	1:D:324:PRO:HD3	2.00	0.43
1:E:20:PRO:HA	1:E:21:PRO:HD3	1.83	0.43
1:E:316:ASP:O	1:E:320:ARG:HG3	2.19	0.43
2:G:6:GLN:N	2:G:114:GLN:HE22	2.17	0.43
3:O:149:VAL:HG11	3:O:179:SER:OG	2.18	0.43
1:C:84:GLN:HA	1:C:84:GLN:NE2	2.33	0.43
1:A:141:VAL:HG12	1:A:210:LYS:HA	2.00	0.43
1:C:73:GLN:CB	1:C:74:PRO:HD2	2.48	0.43
1:C:227:LEU:HD21	1:C:255:THR:HG22	2.01	0.43
1:D:321:ALA:O	1:D:324:PRO:HD2	2.19	0.43
1:E:73:GLN:CB	1:E:74:PRO:HD2	2.49	0.43
1:E:227:LEU:HD21	1:E:255:THR:HG22	2.00	0.43
2:F:36:TRP:CD1	2:F:70:LEU:HD22	2.54	0.43
2:G:36:TRP:CD1	2:G:70:LEU:HD22	2.53	0.43
3:M:154:ASP:OD2	3:M:191:HIS:HB3	2.19	0.43
1:C:103:ILE:HD12	1:C:103:ILE:HA	1.79	0.43
2:H:36:TRP:CD1	2:H:70:LEU:HD22	2.53	0.43
3:L:151:TRP:CZ3	3:L:196:CYS:HB2	2.54	0.43
1:C:163:LYS:O	1:C:167:PRO:HG3	2.18	0.43
1:E:285:THR:CG2	7:E:350:OCT:H21	2.49	0.43
2:G:10:GLU:HG3	2:G:18:MET:CE	2.49	0.43
1:D:302:ASN:HD22	1:E:238:ASP:HB3	1.84	0.42
1:E:34:MET:HG3	1:E:53:LEU:HD12	2.00	0.42
2:J:163:TRP:CZ3	2:J:204:CYS:HB3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLN:CB	1:B:74:PRO:HD2	2.48	0.42
2:F:203:THR:HA	2:F:218:LYS:HA	2.01	0.42
2:J:30:THR:O	2:J:54:TYR:HB2	2.19	0.42
1:B:325:VAL:O	1:B:329:VAL:HG23	2.20	0.42
2:F:164:ASN:CB	2:F:167:SER:HB2	2.49	0.42
2:G:178:VAL:HG22	2:G:185:THR:O	2.18	0.42
2:H:10:GLU:HG3	2:H:18:MET:CE	2.49	0.42
2:J:10:GLU:HG3	2:J:18:MET:CE	2.49	0.42
2:J:36:TRP:CD1	2:J:70:LEU:HD22	2.54	0.42
3:K:111:GLN:HG3	3:K:112:PRO:HD2	2.01	0.42
3:M:201:GLU:O	3:M:201:GLU:HG3	2.19	0.42
2:H:156:PRO:HD2	2:H:210:ALA:HB1	2.02	0.42
2:H:157:GLU:HG3	2:H:184:TYR:CE2	2.54	0.42
2:G:69:THR:HB	2:G:82:GLU:HB2	2.01	0.42
2:G:107:ARG:NH1	3:K:34:PHE:CZ	2.87	0.42
3:K:41:LYS:HB3	3:K:42:PRO:HD2	2.01	0.42
3:K:120:LEU:HD12	3:K:207:LYS:O	2.20	0.42
3:L:153:VAL:O	3:L:153:VAL:HG13	2.19	0.42
1:B:100:LYS:HE2	1:C:104:ASP:H	1.85	0.42
1:C:53:LEU:HD23	1:C:53:LEU:H	1.84	0.42
1:C:194:VAL:HG13	2:G:52:ASN:HB2	2.00	0.42
1:E:325:VAL:O	1:E:329:VAL:HG23	2.19	0.42
2:G:12:VAL:HG21	2:G:86:LEU:HD13	2.02	0.42
2:I:30:THR:O	2:I:54:TYR:HB2	2.19	0.42
2:I:131:TYR:CD1	3:O:126:GLU:OE1	2.73	0.42
3:O:41:LYS:HB3	3:O:42:PRO:HD2	2.01	0.42
1:A:42:ILE:HD12	1:A:181:PHE:CD2	2.54	0.42
1:B:141:VAL:HG12	1:B:210:LYS:HA	2.01	0.42
1:B:316:ASP:O	1:B:320:ARG:HG3	2.19	0.42
1:D:227:LEU:HD21	1:D:255:THR:HG22	2.00	0.42
2:F:10:GLU:HG3	2:F:18:MET:CE	2.49	0.42
2:F:162:THR:OG1	2:F:205:ASN:HB3	2.20	0.42
1:C:274:LYS:HB2	1:C:276:ILE:HG22	2.01	0.42
1:D:36:LEU:HD13	1:D:168:LEU:HD11	2.00	0.42
1:E:274:LYS:HB2	1:E:276:ILE:HG22	2.02	0.42
3:K:120:LEU:HD23	3:K:121:PHE:N	2.35	0.42
1:C:313:LYS:O	1:C:317:LEU:HD13	2.20	0.42
1:D:67:GLY:O	1:D:70:GLY:N	2.50	0.42
1:D:138:PRO:HB2	1:D:139:MET:SD	2.60	0.42
4:D:349:IVM:H1B	4:D:349:IVM:H5	1.84	0.42
2:I:10:GLU:HG3	2:I:18:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:12:VAL:HG21	2:J:86:LEU:HD13	2.02	0.42
1:A:103:ILE:HG23	1:A:103:ILE:O	2.20	0.42
1:B:34:MET:HG3	1:B:53:LEU:HD12	2.01	0.42
1:C:42:ILE:CD1	1:C:209:LEU:HD13	2.50	0.42
3:M:41:LYS:HB3	3:M:42:PRO:HD2	2.02	0.42
1:A:34:MET:CG	1:A:53:LEU:HD12	2.50	0.41
1:A:49:TYR:CE2	1:A:128:LEU:HB2	2.55	0.41
1:C:279:TRP:HB2	1:C:334:TYR:CE1	2.55	0.41
1:E:42:ILE:CD1	1:E:209:LEU:HD13	2.50	0.41
1:E:103:ILE:HG23	1:E:103:ILE:O	2.19	0.41
2:H:6:GLN:N	2:H:114:GLN:HE22	2.16	0.41
2:I:6:GLN:N	2:I:114:GLN:HE22	2.18	0.41
2:I:69:THR:HB	2:I:82:GLU:HB2	2.02	0.41
1:A:226:MET:HB2	4:A:349:IVM:H4B	2.03	0.41
1:B:58:SER:HA	1:B:118:VAL:O	2.21	0.41
1:D:73:GLN:CB	1:D:74:PRO:HD2	2.49	0.41
1:D:284:MET:HG3	1:E:226:MET:HE3	2.01	0.41
1:D:325:VAL:O	1:D:329:VAL:HG23	2.20	0.41
2:G:157:GLU:HG3	2:G:184:TYR:CE2	2.55	0.41
3:K:145:GLY:HA3	3:K:175:TYR:CG	2.55	0.41
1:A:42:ILE:CD1	1:A:209:LEU:HD13	2.49	0.41
1:A:325:VAL:O	1:A:329:VAL:HG23	2.20	0.41
1:C:137:TYR:CE1	1:C:267:LEU:HD21	2.55	0.41
1:C:187:SER:OG	1:C:206:THR:HB	2.20	0.41
1:D:39:ILE:HD13	1:D:207:ILE:HD13	2.01	0.41
1:D:316:ASP:O	1:D:320:ARG:HG3	2.20	0.41
1:E:309:ASN:O	1:E:312:SER:HB3	2.21	0.41
2:F:69:THR:HB	2:F:82:GLU:HB2	2.01	0.41
2:J:159:VAL:HG23	2:J:186:LEU:HD21	2.01	0.41
1:A:58:SER:HA	1:A:118:VAL:O	2.21	0.41
1:A:137:TYR:CE1	1:A:267:LEU:HD21	2.55	0.41
1:A:279:TRP:HB2	1:A:334:TYR:CE1	2.55	0.41
1:C:58:SER:HA	1:C:118:VAL:O	2.21	0.41
1:C:141:VAL:HG12	1:C:210:LYS:HA	2.01	0.41
1:E:58:SER:HA	1:E:118:VAL:O	2.21	0.41
2:F:30:THR:O	2:F:54:TYR:HB2	2.20	0.41
2:G:30:THR:O	2:G:54:TYR:HB2	2.20	0.41
2:J:186:LEU:C	2:J:186:LEU:HD12	2.41	0.41
1:C:138:PRO:HB2	1:C:139:MET:SD	2.59	0.41
1:C:316:ASP:O	1:C:320:ARG:HG3	2.20	0.41
1:C:325:VAL:O	1:C:329:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:TRP:HB2	1:E:334:TYR:CE1	2.56	0.41
1:A:104:ASP:HB3	1:A:105:LYS:H	1.67	0.41
1:D:58:SER:HA	1:D:118:VAL:O	2.21	0.41
2:I:177:ALA:HB2	2:I:186:LEU:HD23	2.02	0.41
3:K:116:PRO:HD3	3:K:200:HIS:ND1	2.36	0.41
3:L:41:LYS:HB3	3:L:42:PRO:HD2	2.02	0.41
3:M:9:ALA:CB	3:M:146:VAL:HG21	2.50	0.41
1:A:194:VAL:HG13	2:H:52:ASN:HB2	2.03	0.41
1:B:67:GLY:O	1:B:70:GLY:N	2.50	0.41
1:B:274:LYS:HB2	1:B:276:ILE:HG22	2.02	0.41
1:C:34:MET:CG	1:C:53:LEU:HD12	2.51	0.41
1:D:161:LEU:HD11	3:O:32:ILE:HG23	2.02	0.41
1:E:104:ASP:HB3	1:E:105:LYS:H	1.67	0.41
2:F:155:PHE:HA	2:F:156:PRO:HA	1.86	0.41
2:H:30:THR:O	2:H:54:TYR:HB2	2.21	0.41
2:H:110:ASP:HB3	2:H:111:TYR:HD2	1.86	0.41
3:M:87:ILE:HD11	3:M:105:LYS:HE2	2.02	0.41
3:M:170:GLN:HE21	3:M:172:ASN:HD21	1.68	0.41
1:A:187:SER:OG	1:A:206:THR:HB	2.20	0.41
1:B:187:SER:OG	1:B:206:THR:HB	2.21	0.41
1:B:286:PHE:CZ	7:B:351:OCT:H42	2.55	0.41
4:B:349:IVM:H14	4:B:349:IVM:H1B	2.03	0.41
1:C:49:TYR:CE2	1:C:128:LEU:HB2	2.56	0.41
1:E:137:TYR:CE1	1:E:267:LEU:HD21	2.56	0.41
2:F:12:VAL:HG21	2:F:86:LEU:HD13	2.02	0.41
2:H:159:VAL:HG23	2:H:186:LEU:HD21	2.02	0.41
2:J:69:THR:HB	2:J:82:GLU:HB2	2.01	0.41
3:L:130:THR:O	3:L:130:THR:HG22	2.21	0.41
3:L:152:LYS:HD3	3:L:197:GLN:HE21	1.84	0.41
3:M:123:PRO:HD2	3:M:188:TRP:CZ2	2.56	0.41
1:A:274:LYS:HB2	1:A:276:ILE:HG22	2.03	0.41
1:D:49:TYR:CE2	1:D:128:LEU:HB2	2.56	0.41
1:D:328:PHE:CE2	1:D:332:ILE:HD11	2.56	0.41
2:F:46:GLU:OE1	2:F:63:LYS:HE2	2.21	0.41
2:F:110:ASP:HB3	2:F:111:TYR:HD2	1.86	0.41
2:G:110:ASP:HB3	2:G:111:TYR:HD2	1.85	0.41
2:H:69:THR:HB	2:H:82:GLU:HB2	2.02	0.41
2:I:175:PHE:HB3	2:I:176:PRO:HD2	2.03	0.41
2:J:197:TRP:CH2	2:J:221:PRO:HD3	2.56	0.41
3:L:139:ILE:HG12	3:L:177:ALA:O	2.20	0.41
3:N:36:ASN:O	3:N:90:CYS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:130:THR:HG22	3:O:130:THR:O	2.20	0.41
1:B:313:LYS:O	1:B:317:LEU:HD13	2.20	0.41
2:J:126:THR:HA	2:J:127:PRO:HD2	1.94	0.41
2:J:155:PHE:HA	2:J:156:PRO:HA	1.86	0.41
3:K:87:ILE:HD11	3:K:105:LYS:HE2	2.03	0.41
1:A:316:ASP:O	1:A:320:ARG:HG3	2.20	0.40
1:B:20:PRO:HD3	1:B:86:TRP:CD2	2.56	0.40
1:B:49:TYR:CE2	1:B:128:LEU:HB2	2.56	0.40
1:B:103:ILE:O	1:B:103:ILE:HG23	2.19	0.40
1:D:90:THR:HG22	1:D:160:TYR:HH	1.82	0.40
1:E:267:LEU:HD13	1:E:274:LYS:HE3	2.03	0.40
2:J:6:GLN:N	2:J:114:GLN:HE22	2.19	0.40
3:L:123:PRO:HD3	3:L:135:LEU:HD13	2.02	0.40
3:M:145:GLY:HA3	3:M:175:TYR:CG	2.55	0.40
1:A:49:TYR:CZ	1:A:128:LEU:HD12	2.56	0.40
1:A:222:ILE:HG23	4:A:349:IVM:H2A	2.02	0.40
1:B:246:VAL:HG21	1:C:244:ALA:HB1	2.03	0.40
4:C:350:IVM:H14	4:C:350:IVM:H1B	2.03	0.40
1:D:137:TYR:CE1	1:D:267:LEU:HD21	2.56	0.40
1:E:313:LYS:O	1:E:317:LEU:HD13	2.20	0.40
2:G:131:TYR:CD1	3:K:127:GLU:HB3	2.56	0.40
3:K:109:LEU:CD2	3:K:143:TYR:HE2	2.34	0.40
3:M:170:GLN:NE2	3:M:172:ASN:HD21	2.19	0.40
3:O:87:ILE:HD11	3:O:105:LYS:HE2	2.03	0.40
1:D:187:SER:OG	1:D:206:THR:HB	2.22	0.40
1:D:274:LYS:HB2	1:D:276:ILE:HG22	2.02	0.40
4:E:349:IVM:H14	4:E:349:IVM:H1B	2.03	0.40
3:K:36:ASN:O	3:K:90:CYS:HA	2.22	0.40
3:K:162:MET:C	3:K:163:GLU:HG3	2.42	0.40
3:L:36:ASN:O	3:L:90:CYS:HA	2.21	0.40
3:L:105:LYS:HE3	3:L:105:LYS:HB2	1.93	0.40
3:O:131:ASN:HA	3:O:185:ALA:HB2	2.03	0.40
4:A:349:IVM:O12	1:E:284:MET:HG2	2.22	0.40
1:C:103:ILE:HG23	1:C:103:ILE:O	2.20	0.40
2:F:6:GLN:N	2:F:114:GLN:HE22	2.18	0.40
2:H:213:THR:HG22	2:H:215:VAL:HG13	2.04	0.40
2:J:208:HIS:HB3	2:J:213:THR:HB	2.03	0.40
3:M:204:THR:HG22	3:M:205:VAL:N	2.36	0.40
1:A:20:PRO:HD3	1:A:86:TRP:CD2	2.56	0.40
1:D:224:SER:CB	1:D:279:TRP:CH2	3.03	0.40
1:E:34:MET:CG	1:E:53:LEU:HD12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:SER:OG	1:E:206:THR:HB	2.21	0.40
4:E:349:IVM:H1B	4:E:349:IVM:H5	1.84	0.40
2:H:46:GLU:OE1	2:H:63:LYS:HE2	2.22	0.40
2:H:128:PRO:HB2	2:H:151:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/347 (97%)	318 (94%)	18 (5%)	2 (1%)	25	57
1	B	338/347 (97%)	316 (94%)	20 (6%)	2 (1%)	25	57
1	C	337/347 (97%)	316 (94%)	19 (6%)	2 (1%)	25	57
1	D	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	25	57
1	E	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	25	57
2	F	182/221 (82%)	169 (93%)	12 (7%)	1 (0%)	29	61
2	G	194/221 (88%)	179 (92%)	14 (7%)	1 (0%)	29	61
2	H	219/221 (99%)	204 (93%)	15 (7%)	0	100	100
2	I	193/221 (87%)	181 (94%)	10 (5%)	2 (1%)	15	46
2	J	211/221 (96%)	197 (93%)	14 (7%)	0	100	100
3	K	195/210 (93%)	176 (90%)	18 (9%)	1 (0%)	29	61
3	L	208/210 (99%)	191 (92%)	16 (8%)	1 (0%)	29	61
3	M	208/210 (99%)	192 (92%)	16 (8%)	0	100	100
3	N	148/210 (70%)	133 (90%)	15 (10%)	0	100	100
3	O	189/210 (90%)	166 (88%)	23 (12%)	0	100	100
All	All	3636/3890 (94%)	3372 (93%)	248 (7%)	16 (0%)	34	67

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	190	VAL
1	A	68	VAL
1	B	68	VAL
1	C	68	VAL
1	D	68	VAL
1	E	68	VAL
2	G	28	SER
3	L	109	LEU
1	A	137	TYR
1	B	137	TYR
1	C	137	TYR
1	D	137	TYR
1	E	137	TYR
2	F	178	VAL
2	I	178	VAL
3	K	146	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/316 (97%)	304 (99%)	3 (1%)	76	88
1	B	307/316 (97%)	304 (99%)	3 (1%)	76	88
1	C	306/316 (97%)	303 (99%)	3 (1%)	76	88
1	D	307/316 (97%)	304 (99%)	3 (1%)	76	88
1	E	307/316 (97%)	303 (99%)	4 (1%)	69	84
2	F	158/190 (83%)	158 (100%)	0	100	100
2	G	171/190 (90%)	170 (99%)	1 (1%)	86	94
2	H	190/190 (100%)	190 (100%)	0	100	100
2	I	172/190 (90%)	172 (100%)	0	100	100
2	J	185/190 (97%)	185 (100%)	0	100	100
3	K	169/178 (95%)	168 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	178/178 (100%)	175 (98%)	3 (2%)	60	80
3	M	176/178 (99%)	175 (99%)	1 (1%)	86	94
3	N	128/178 (72%)	128 (100%)	0	100	100
3	O	162/178 (91%)	161 (99%)	1 (1%)	86	94
All	All	3223/3420 (94%)	3200 (99%)	23 (1%)	84	92

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	A	104	ASP
1	A	189	THR
1	B	95	GLU
1	B	104	ASP
1	B	189	THR
1	C	95	GLU
1	C	104	ASP
1	C	189	THR
1	D	95	GLU
1	D	104	ASP
1	D	189	THR
1	E	95	GLU
1	E	104	ASP
1	E	189	THR
1	E	292	LEU
2	G	45	LEU
3	K	141	ASP
3	L	118	VAL
3	L	149	VAL
3	L	189	GLU
3	M	109	LEU
3	O	3	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	264	ASN
1	A	299	HIS
1	B	46	ASN

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Mol	Chain	Res	Type
1	B	84	GLN
1	B	264	ASN
1	C	84	GLN
1	C	264	ASN
1	D	46	ASN
1	D	84	GLN
1	D	169	GLN
1	D	264	ASN
1	E	84	GLN
1	E	264	ASN
2	F	5	GLN
2	F	62	GLN
2	F	173	HIS
2	F	180	GLN
2	F	208	HIS
2	G	5	GLN
2	G	62	GLN
2	H	5	GLN
2	H	62	GLN
2	H	180	GLN
2	I	5	GLN
2	I	62	GLN
2	I	180	GLN
2	J	5	GLN
2	J	62	GLN
3	K	111	GLN
3	K	197	GLN
3	L	197	GLN
3	M	160	GLN
3	M	166	GLN
3	M	172	ASN
3	N	166	GLN
3	N	170	GLN
3	O	166	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	C	400	1	14,14,15	0.37	0	17,19,21	1.92	2 (11%)
7	OCT	D	350	-	7,7,7	0.28	0	6,6,6	0.38	0
8	UND	B	352	-	10,10,10	0.31	0	9,9,9	0.37	0
4	IVM	D	349	-	65,68,68	0.80	1 (1%)	82,102,102	1.63	16 (19%)
4	IVM	E	349	-	65,68,68	0.81	1 (1%)	82,102,102	1.64	18 (21%)
5	LMT	A	351	-	28,28,36	1.47	4 (14%)	39,39,47	1.37	5 (12%)
4	IVM	C	350	-	65,68,68	0.82	1 (1%)	82,102,102	1.61	17 (20%)
10	RI5	E	351	-	23,25,25	2.40	6 (26%)	26,46,46	2.20	10 (38%)
4	IVM	A	349	-	65,68,68	0.79	1 (1%)	82,102,102	1.62	17 (20%)
5	LMT	B	350	-	27,27,36	1.54	4 (14%)	37,38,47	1.41	5 (13%)
7	OCT	E	350	-	7,7,7	0.28	0	6,6,6	0.42	0
7	OCT	B	351	-	7,7,7	0.25	0	6,6,6	0.41	0
4	IVM	B	349	-	65,68,68	0.79	1 (1%)	82,102,102	1.62	17 (20%)
6	NAG	B	400	1	14,14,15	0.52	0	17,19,21	0.97	2 (11%)
5	LMT	A	350	-	27,27,36	1.50	4 (14%)	37,38,47	1.81	9 (24%)
6	NAG	E	400	1	14,14,15	0.49	0	17,19,21	1.42	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	400	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OCT	D	350	-	-	0/5/5/5	-
8	UND	B	352	-	-	0/8/8/8	-
4	IVM	D	349	-	-	6/45/141/141	0/6/7/7
4	IVM	E	349	-	-	6/45/141/141	0/6/7/7
5	LMT	A	351	-	-	6/13/53/61	0/2/2/2
4	IVM	C	350	-	-	6/45/141/141	0/6/7/7
10	RI5	E	351	-	-	3/4/77/77	0/6/5/5
4	IVM	A	349	-	-	6/45/141/141	0/6/7/7
5	LMT	B	350	-	-	7/12/52/61	0/2/2/2
7	OCT	E	350	-	-	0/5/5/5	-
7	OCT	B	351	-	-	0/5/5/5	-
4	IVM	B	349	-	-	6/45/141/141	0/6/7/7
6	NAG	B	400	1	-	0/6/23/26	0/1/1/1
5	LMT	A	350	-	-	7/12/52/61	0/2/2/2
6	NAG	E	400	1	-	4/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	351	RI5	O12-C10	6.85	1.45	1.35
10	E	351	RI5	O19-C17	6.56	1.45	1.35
4	C	350	IVM	O12-C46	4.95	1.45	1.34
4	E	349	IVM	O12-C46	4.85	1.45	1.34
4	B	349	IVM	O12-C46	4.83	1.45	1.34
4	D	349	IVM	O12-C46	4.78	1.45	1.34
4	A	349	IVM	O12-C46	4.69	1.45	1.34
5	B	350	LMT	C3'-C4'	-4.01	1.41	1.52
5	A	350	LMT	C3'-C4'	-3.87	1.42	1.52
5	A	351	LMT	C3'-C4'	-3.83	1.42	1.52
5	B	350	LMT	C4B-C3B	-3.81	1.42	1.52
5	A	350	LMT	C4B-C3B	-3.68	1.42	1.52
5	A	351	LMT	C4B-C3B	-3.62	1.43	1.52
5	A	351	LMT	C3B-C2B	-2.86	1.45	1.52
5	B	350	LMT	C3B-C2B	-2.84	1.45	1.52
10	E	351	RI5	O12-C05	-2.78	1.42	1.46
10	E	351	RI5	C08-C07	-2.74	1.52	1.57
5	A	350	LMT	C3B-C2B	-2.61	1.45	1.52
10	E	351	RI5	C08-C09	-2.51	1.52	1.55
10	E	351	RI5	C15-C14	2.42	1.52	1.48
5	B	350	LMT	O2'-C2'	-2.22	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	351	LMT	O2'-C2'	-2.22	1.37	1.43
5	A	350	LMT	O2'-C2'	-2.12	1.38	1.43

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	349	IVM	O12-C46-C45	6.72	120.69	110.97
4	A	349	IVM	O12-C46-C45	6.71	120.69	110.97
4	D	349	IVM	O12-C46-C45	6.63	120.56	110.97
4	C	350	IVM	O12-C46-C45	6.54	120.43	110.97
4	B	349	IVM	O12-C46-C45	6.44	120.30	110.97
6	C	400	NAG	C1-O5-C5	6.36	120.80	112.19
10	E	351	RI5	C05-O12-C10	-5.32	102.35	109.87
4	D	349	IVM	C13-C14-C15	-4.60	107.04	113.21
4	C	350	IVM	C13-C14-C15	-4.59	107.05	113.21
4	B	349	IVM	C13-C14-C15	-4.57	107.08	113.21
4	E	349	IVM	C13-C14-C15	-4.52	107.15	113.21
5	A	350	LMT	C1B-O5B-C5B	-4.46	104.92	113.69
4	A	349	IVM	C13-C14-C15	-4.30	107.45	113.21
6	C	400	NAG	O5-C1-C2	3.79	117.28	111.29
4	D	349	IVM	O9-C40-C39	-3.66	102.35	105.73
10	E	351	RI5	O16-C15-C07	3.66	122.95	115.32
4	A	349	IVM	O9-C40-C39	-3.51	102.49	105.73
4	E	349	IVM	O9-C40-C39	-3.45	102.54	105.73
4	C	350	IVM	O9-C40-C39	-3.40	102.59	105.73
6	E	400	NAG	C1-O5-C5	3.39	116.78	112.19
5	B	350	LMT	C1-O1'-C1'	3.38	119.45	113.84
4	B	349	IVM	O9-C40-C39	-3.36	102.63	105.73
5	A	350	LMT	C1-O1'-C1'	3.33	119.36	113.84
10	E	351	RI5	C13-C08-C07	3.27	107.49	103.24
10	E	351	RI5	C04-C09-C10	-3.26	97.64	103.35
5	A	351	LMT	O3'-C3'-C2'	-3.18	102.99	110.35
5	A	351	LMT	C1-O1'-C1'	3.13	119.03	113.84
5	A	350	LMT	O1B-C1B-O5B	-3.06	102.13	110.67
4	A	349	IVM	C12-O12-C46	-3.00	112.78	117.69
4	E	349	IVM	C12-O12-C46	-2.96	112.84	117.69
4	D	349	IVM	C12-O12-C46	-2.92	112.91	117.69
4	D	349	IVM	C3-C5-C9	-2.91	111.29	116.50
10	E	351	RI5	O11-C10-C09	-2.91	125.45	129.53
5	A	350	LMT	C2'-C3'-C4'	2.90	116.30	109.68
4	C	350	IVM	C12-O12-C46	-2.89	112.95	117.69
4	E	349	IVM	C3-C5-C9	-2.86	111.38	116.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	349	IVM	O12-C46-O11	-2.85	118.62	123.94
4	B	349	IVM	C12-O12-C46	-2.84	113.03	117.69
4	C	350	IVM	C3-C5-C9	-2.83	111.44	116.50
5	B	350	LMT	O3'-C3'-C2'	-2.83	103.81	110.35
4	B	349	IVM	C3-C5-C9	-2.80	111.49	116.50
4	A	349	IVM	O12-C46-O11	-2.80	118.71	123.94
4	A	349	IVM	C3-C5-C9	-2.78	111.53	116.50
4	B	349	IVM	O1-C5-C3	2.77	110.34	106.12
4	E	349	IVM	O11-C46-C45	-2.77	120.31	125.05
10	E	351	RI5	O12-C10-C09	2.74	112.74	109.82
4	D	349	IVM	O1-C5-C3	2.73	110.29	106.12
4	A	349	IVM	O1-C5-C3	2.69	110.21	106.12
5	A	350	LMT	O3'-C3'-C2'	-2.67	104.17	110.35
4	E	349	IVM	O12-C46-O11	-2.66	118.97	123.94
4	C	350	IVM	O12-C46-O11	-2.66	118.97	123.94
4	B	349	IVM	C15-C16-C17	-2.66	120.96	127.56
10	E	351	RI5	C13-C14-C15	-2.65	105.07	108.70
5	A	350	LMT	O1B-C4'-C3'	-2.63	100.29	107.28
4	D	349	IVM	C15-C16-C17	-2.63	121.04	127.56
4	E	349	IVM	C15-C16-C17	-2.62	121.05	127.56
4	E	349	IVM	C37-C38-C39	-2.62	121.78	130.07
4	C	350	IVM	O11-C46-C45	-2.62	120.57	125.05
4	C	350	IVM	C34-C19-C17	-2.62	108.67	113.89
4	A	349	IVM	C15-C16-C17	-2.62	121.07	127.56
4	B	349	IVM	O11-C46-C45	-2.62	120.57	125.05
4	A	349	IVM	O11-C46-C45	-2.61	120.57	125.05
10	E	351	RI5	C15-O16-C14	2.60	64.35	61.53
4	B	349	IVM	O12-C46-O11	-2.59	119.10	123.94
4	E	349	IVM	C34-C19-C17	-2.59	108.73	113.89
5	A	350	LMT	O1B-C1B-C2B	2.58	114.78	108.10
4	C	350	IVM	O1-C5-C3	2.58	110.05	106.12
5	A	351	LMT	O1'-C1-C2	2.57	118.56	109.56
4	C	350	IVM	C15-C16-C17	-2.57	121.19	127.56
4	D	349	IVM	C37-C38-C39	-2.56	121.98	130.07
4	B	349	IVM	C34-C19-C17	-2.56	108.79	113.89
4	B	349	IVM	C37-C38-C39	-2.55	122.01	130.07
4	E	349	IVM	O1-C5-C3	2.53	109.98	106.12
5	A	350	LMT	O3B-C3B-C4B	-2.53	104.50	110.35
4	D	349	IVM	C34-C19-C17	-2.51	108.89	113.89
4	A	349	IVM	C38-C37-C36	-2.50	118.46	124.53
4	A	349	IVM	C37-C38-C39	-2.50	122.18	130.07
4	D	349	IVM	O11-C46-C45	-2.49	120.79	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	349	IVM	C38-C37-C36	-2.48	118.52	124.53
6	B	400	NAG	C1-O5-C5	2.47	115.54	112.19
4	C	350	IVM	C37-C38-C39	-2.47	122.27	130.07
4	E	349	IVM	C38-C37-C36	-2.44	118.60	124.53
4	B	349	IVM	O14-C14-C13	2.42	113.49	108.94
4	B	349	IVM	C38-C37-C36	-2.42	118.66	124.53
4	A	349	IVM	C34-C19-C17	-2.42	109.07	113.89
4	C	350	IVM	C38-C37-C36	-2.42	118.67	124.53
4	C	350	IVM	O14-C14-C15	2.41	108.14	105.82
5	B	350	LMT	O1B-C1B-C2B	2.39	114.30	108.10
5	B	350	LMT	C1B-O1B-C4'	-2.38	112.07	117.96
5	B	350	LMT	O3B-C3B-C4B	-2.38	104.85	110.35
4	E	349	IVM	O14-C14-C13	2.38	113.41	108.94
4	B	349	IVM	O14-C14-C15	2.37	108.11	105.82
10	E	351	RI5	O19-C17-O18	2.35	124.73	121.62
5	A	351	LMT	C1B-O1B-C4'	-2.34	112.17	117.96
4	D	349	IVM	O14-C14-C13	2.32	113.30	108.94
4	A	349	IVM	C18-C17-C19	2.31	119.68	115.68
4	E	349	IVM	O14-C14-C15	2.30	108.03	105.82
4	A	349	IVM	O14-C14-C13	2.29	113.25	108.94
5	A	350	LMT	O5B-C5B-C6B	2.28	112.10	106.44
6	E	400	NAG	C2-N2-C7	2.27	126.14	122.90
4	C	350	IVM	C18-C17-C19	2.27	119.60	115.68
4	D	349	IVM	C18-C17-C19	2.24	119.55	115.68
4	B	349	IVM	C18-C17-C19	2.23	119.54	115.68
4	C	350	IVM	C8-C9-C5	2.23	111.78	108.41
4	E	349	IVM	C18-C17-C19	2.22	119.52	115.68
10	E	351	RI5	O18-C17-C15	-2.21	126.33	129.09
4	C	350	IVM	O14-C14-C13	2.21	113.09	108.94
4	E	349	IVM	C8-C9-C5	2.19	111.72	108.41
4	A	349	IVM	O14-C14-C15	2.19	107.93	105.82
4	D	349	IVM	O14-C14-C15	2.13	107.88	105.82
4	D	349	IVM	C8-C9-C5	2.12	111.62	108.41
4	B	349	IVM	C8-C9-C5	2.10	111.59	108.41
4	B	349	IVM	C48-C43-C44	-2.10	119.07	123.56
4	E	349	IVM	C48-C43-C44	-2.09	119.09	123.56
6	B	400	NAG	O5-C1-C2	2.07	114.56	111.29
4	A	349	IVM	C8-C9-C5	2.07	111.53	108.41
4	E	349	IVM	C7-C6-C11	-2.06	108.98	112.55
4	C	350	IVM	C6-O1-C5	-2.02	111.47	114.27
5	A	351	LMT	O6'-C6'-C5'	2.02	118.22	111.29
4	A	349	IVM	C34-C36-C37	-2.01	121.92	126.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	400	NAG	C1-C2-N2	2.01	113.92	110.49
6	E	400	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	349	IVM	O7-C25-O4-C24
4	A	349	IVM	C26-C25-O4-C24
4	B	349	IVM	O7-C25-O4-C24
4	B	349	IVM	C26-C25-O4-C24
4	C	350	IVM	O7-C25-O4-C24
4	C	350	IVM	C26-C25-O4-C24
4	D	349	IVM	O7-C25-O4-C24
4	D	349	IVM	C26-C25-O4-C24
4	E	349	IVM	O7-C25-O4-C24
4	E	349	IVM	C26-C25-O4-C24
5	A	351	LMT	C2'-C1'-O1'-C1
5	A	351	LMT	O5'-C1'-O1'-C1
6	E	400	NAG	O7-C7-N2-C2
6	E	400	NAG	C8-C7-N2-C2
5	A	350	LMT	O5B-C1B-O1B-C4'
5	B	350	LMT	C2B-C1B-O1B-C4'
5	B	350	LMT	O5B-C1B-O1B-C4'
5	B	350	LMT	O5'-C5'-C6'-O6'
5	A	350	LMT	O5'-C5'-C6'-O6'
5	A	350	LMT	C3'-C4'-O1B-C1B
6	E	400	NAG	C1-C2-N2-C7
5	A	351	LMT	O5'-C5'-C6'-O6'
5	A	350	LMT	O5B-C5B-C6B-O6B
5	A	350	LMT	C2B-C1B-O1B-C4'
5	A	351	LMT	O1'-C1-C2-C3
5	A	350	LMT	C5'-C4'-O1B-C1B
6	E	400	NAG	O5-C5-C6-O6
5	B	350	LMT	O5B-C5B-C6B-O6B
5	B	350	LMT	C4'-C5'-C6'-O6'
4	A	349	IVM	C19-C34-C36-C37
4	B	349	IVM	C19-C34-C36-C37
4	C	350	IVM	C19-C34-C36-C37
4	D	349	IVM	C19-C34-C36-C37
4	E	349	IVM	C19-C34-C36-C37
4	B	349	IVM	O11-C46-O12-C12

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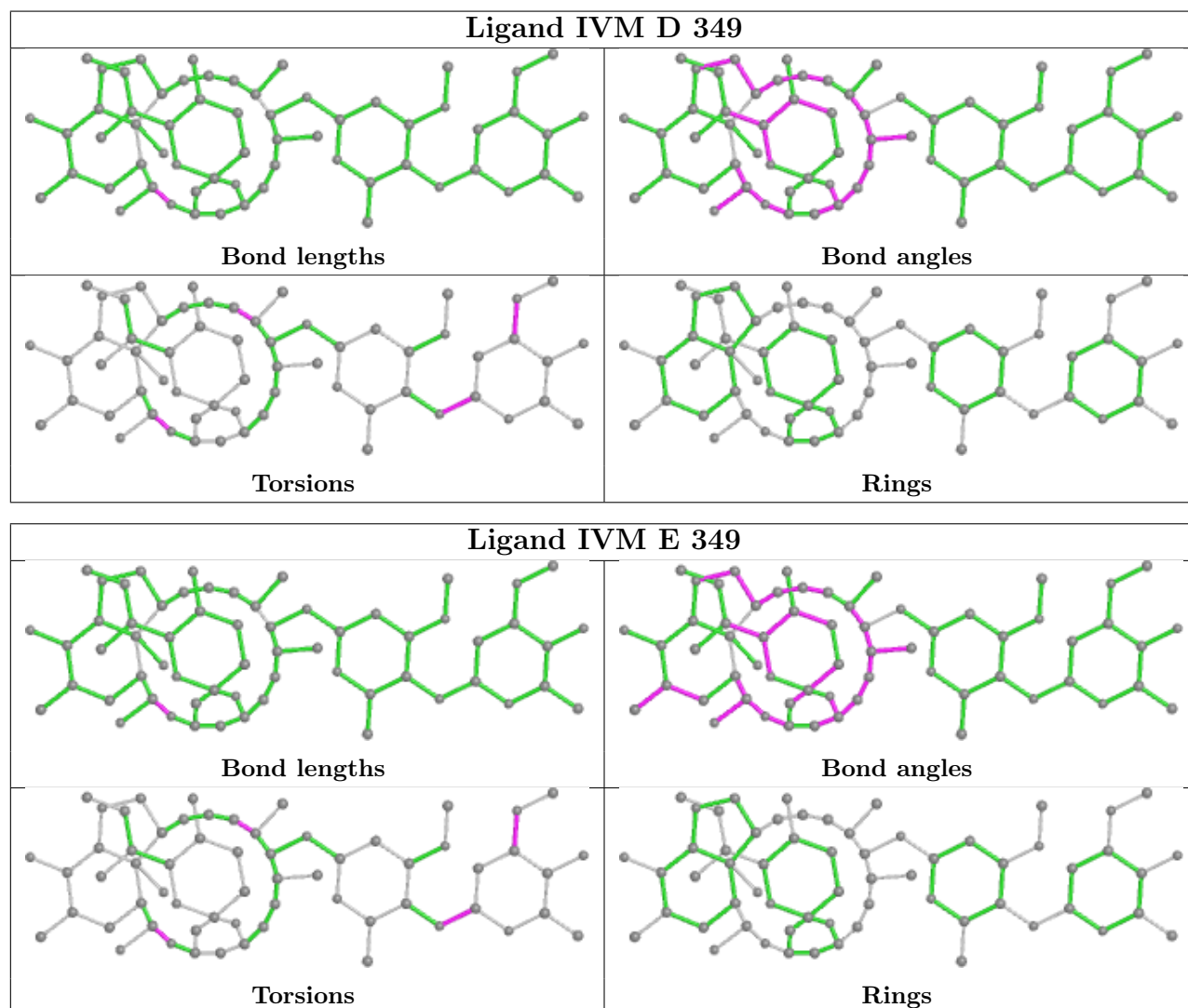
Mol	Chain	Res	Type	Atoms
4	C	350	IVM	O11-C46-O12-C12
5	B	350	LMT	O1'-C1-C2-C3
4	A	349	IVM	O11-C46-O12-C12
4	D	349	IVM	O11-C46-O12-C12
4	E	349	IVM	O11-C46-O12-C12
4	B	349	IVM	C45-C46-O12-C12
5	A	350	LMT	C4'-C5'-C6'-O6'
10	E	351	RI5	C03-C02-C04-C05
10	E	351	RI5	C01-C02-C04-C05
4	A	349	IVM	C45-C46-O12-C12
4	C	350	IVM	C45-C46-O12-C12
4	E	349	IVM	C45-C46-O12-C12
4	A	349	IVM	C26-C27-O5-C28
4	B	349	IVM	C26-C27-O5-C28
4	C	350	IVM	C26-C27-O5-C28
4	D	349	IVM	C26-C27-O5-C28
4	E	349	IVM	C26-C27-O5-C28
4	D	349	IVM	C45-C46-O12-C12
10	E	351	RI5	C01-C02-C04-C09
5	A	351	LMT	C2B-C1B-O1B-C4'
5	A	351	LMT	C1-C2-C3-C4
5	B	350	LMT	C2-C1-O1'-C1'

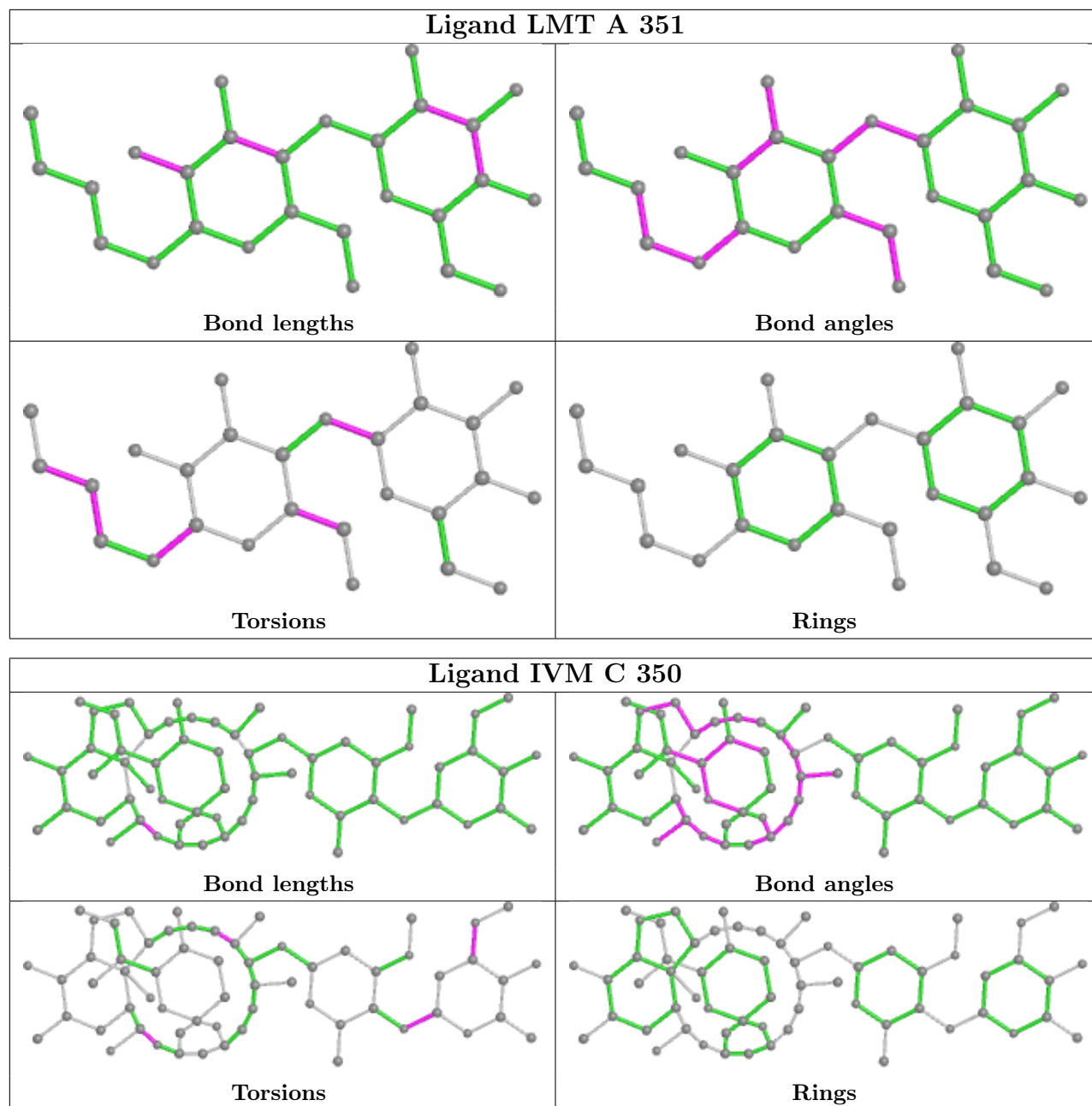
There are no ring outliers.

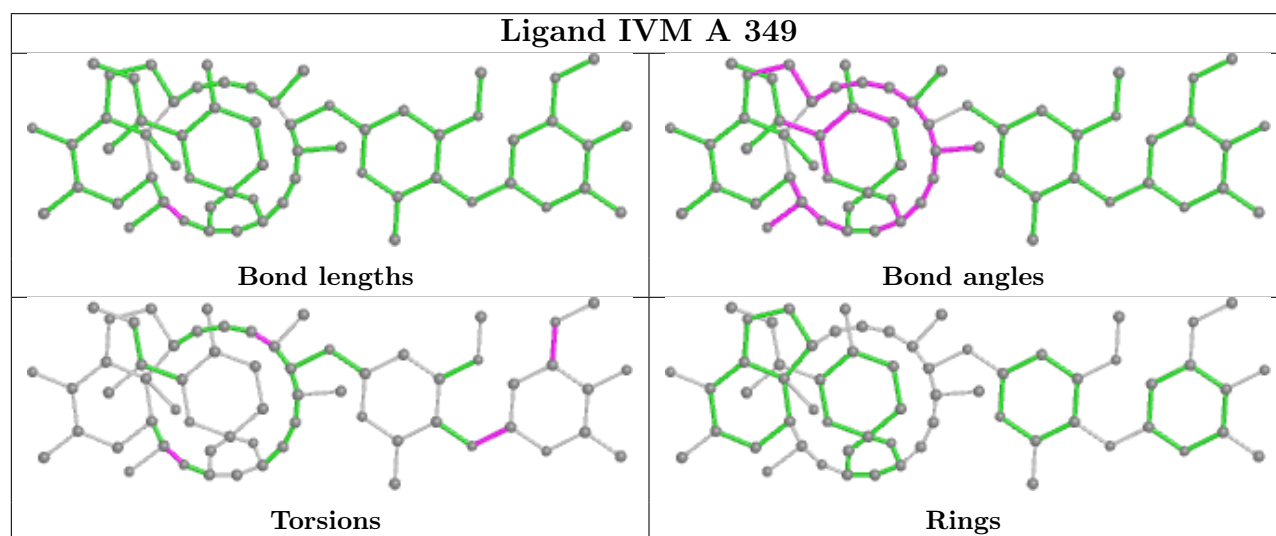
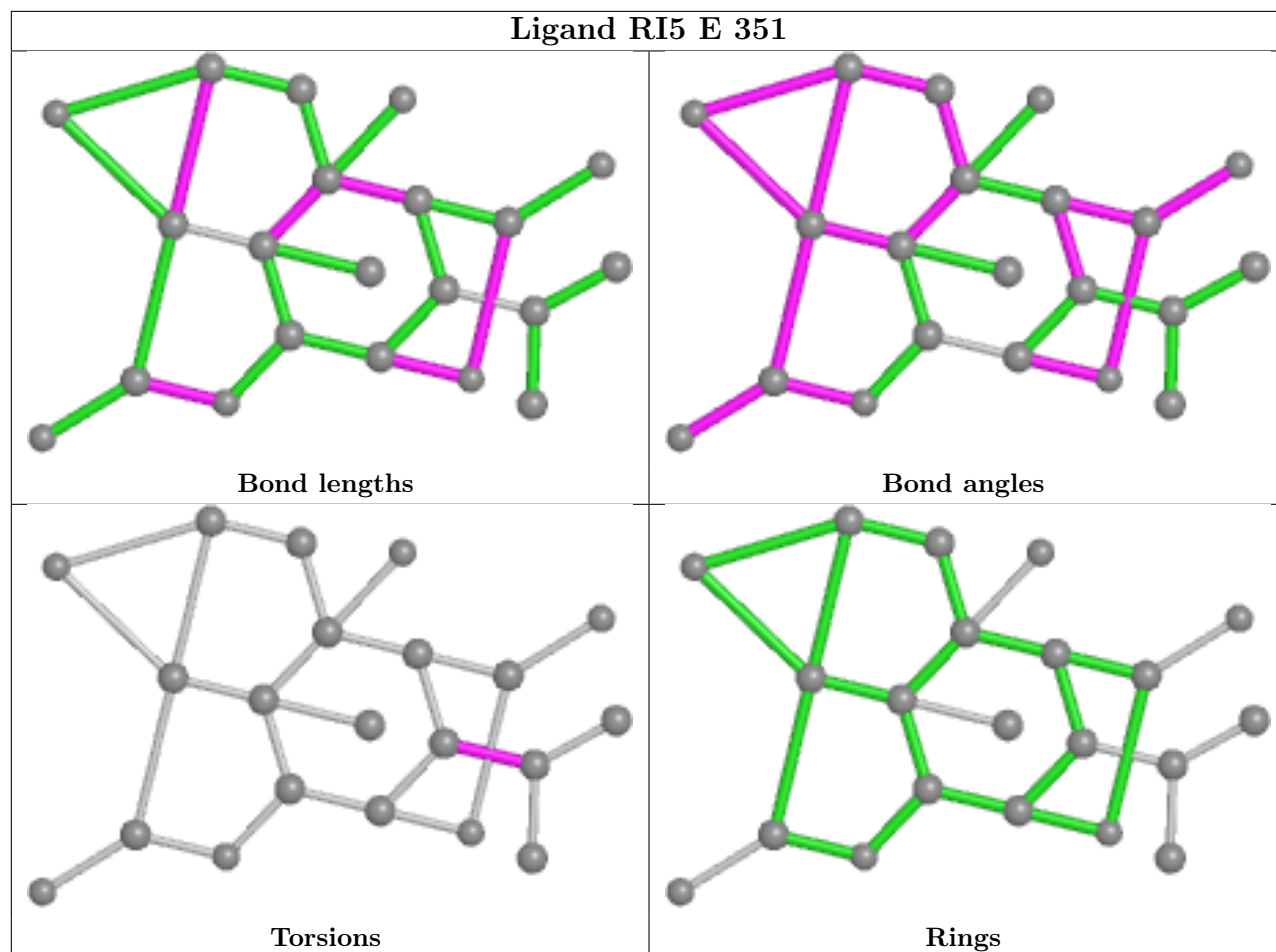
14 monomers are involved in 63 short contacts:

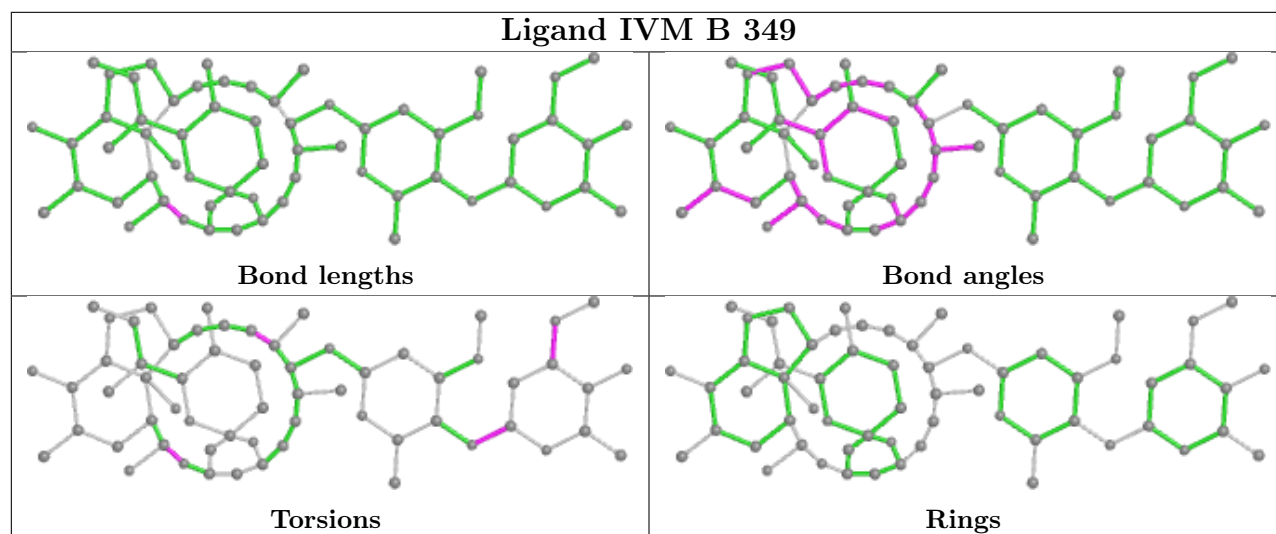
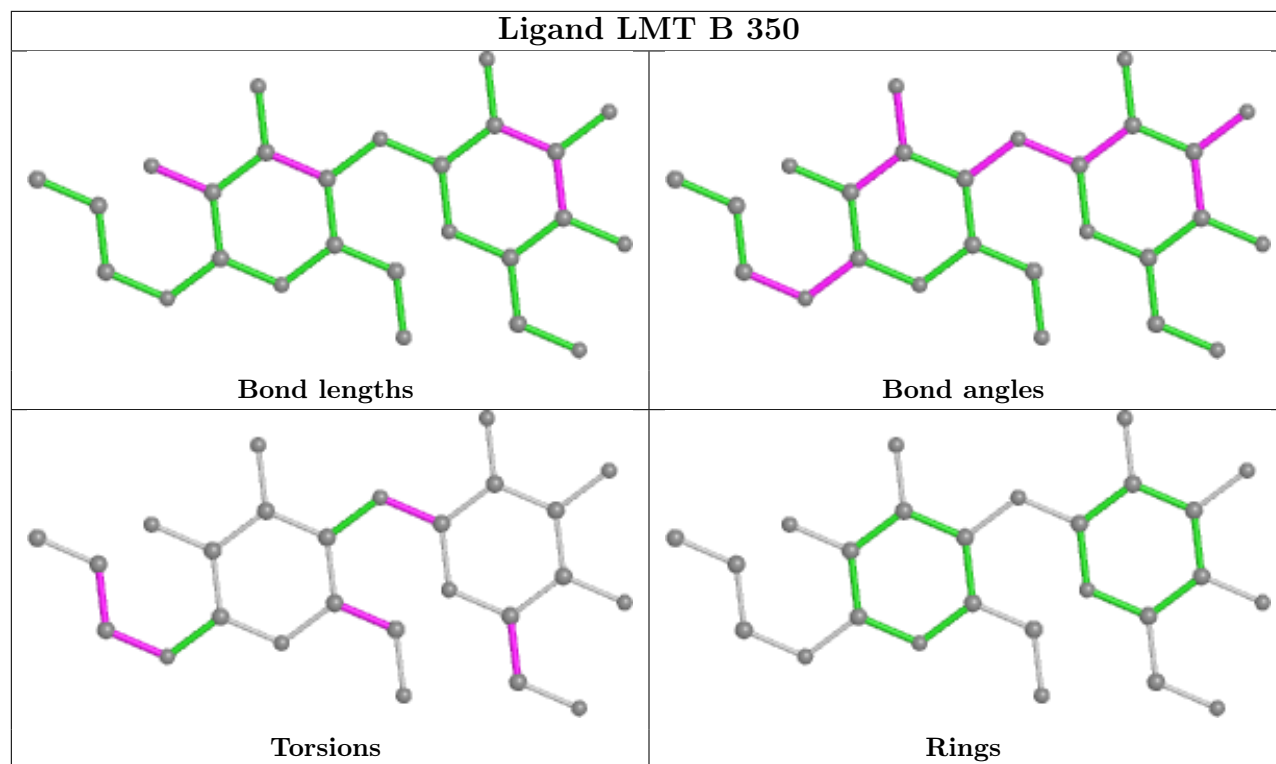
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	400	NAG	1	0
7	D	350	OCT	1	0
4	D	349	IVM	3	0
4	E	349	IVM	7	0
5	A	351	LMT	3	0
4	C	350	IVM	5	0
10	E	351	RI5	15	0
4	A	349	IVM	5	0
5	B	350	LMT	5	0
7	E	350	OCT	3	0
7	B	351	OCT	1	0
4	B	349	IVM	2	0
6	B	400	NAG	1	0
5	A	350	LMT	11	0

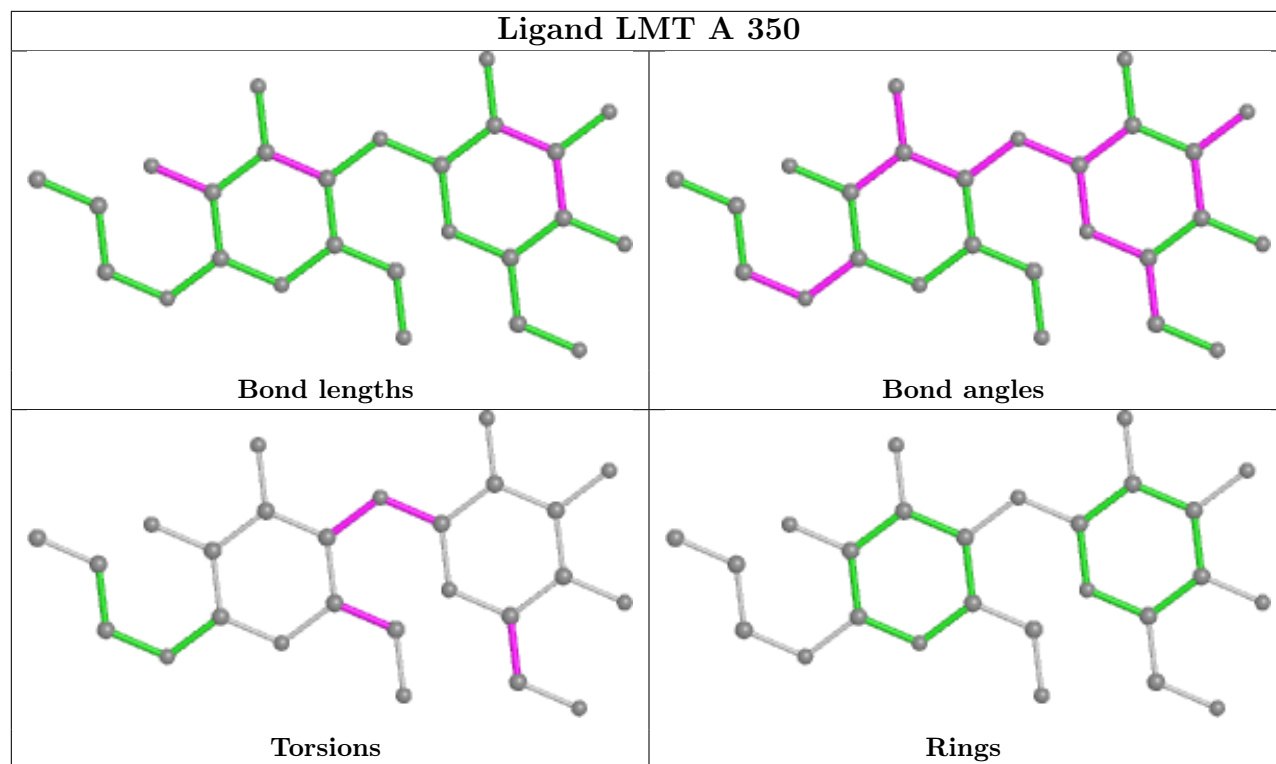
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	340/347 (97%)	-0.03	1 (0%) 94 93	42, 72, 125, 179	0
1	B	340/347 (97%)	-0.05	4 (1%) 79 77	47, 74, 129, 206	0
1	C	339/347 (97%)	0.06	10 (2%) 51 50	42, 76, 143, 234	0
1	D	340/347 (97%)	-0.07	4 (1%) 79 77	44, 80, 144, 252	0
1	E	340/347 (97%)	-0.04	3 (0%) 84 83	41, 76, 150, 230	0
2	F	188/221 (85%)	0.78	29 (15%) 2 2	59, 112, 184, 237	0
2	G	200/221 (90%)	0.44	14 (7%) 16 18	60, 99, 145, 177	0
2	H	221/221 (100%)	0.01	1 (0%) 91 90	47, 82, 139, 257	0
2	I	199/221 (90%)	0.79	34 (17%) 1 2	63, 112, 174, 207	0
2	J	215/221 (97%)	0.22	8 (3%) 41 40	55, 89, 149, 212	0
3	K	199/210 (94%)	0.13	5 (2%) 57 55	67, 107, 151, 198	0
3	L	210/210 (100%)	0.08	2 (0%) 82 81	44, 81, 129, 171	0
3	M	210/210 (100%)	0.07	2 (0%) 82 81	55, 92, 133, 197	0
3	N	158/210 (75%)	1.27	51 (32%) 0 0	65, 121, 197, 232	0
3	O	195/210 (92%)	0.72	22 (11%) 5 6	69, 117, 170, 218	0
All	All	3694/3890 (94%)	0.22	190 (5%) 28 28	41, 87, 159, 257	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	208	SER	7.5
2	J	137	SER	7.3
3	N	109	LEU	6.7
1	B	302	ASN	5.9
2	I	189	SER	5.6
2	F	132	PRO	5.5
3	N	165	THR	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	308	TRP	5.3
2	F	187	SER	5.2
3	N	135	LEU	5.1
3	N	120	LEU	5.1
3	N	178	SER	5.0
2	I	188	SER	4.9
2	F	168	LEU	4.7
2	I	195	SER	4.6
2	G	168	LEU	4.6
2	F	178	VAL	4.6
2	F	131	TYR	4.5
2	F	150	LEU	4.4
3	O	207	LYS	4.4
1	C	304	GLY	4.4
1	E	340	HIS	4.3
3	L	1	GLN	4.3
3	N	122	PRO	4.3
3	N	108	VAL	4.3
2	F	186	LEU	4.2
3	N	136	VAL	4.2
1	C	305	THR	4.2
3	N	144	PRO	4.1
2	F	170	SER	4.1
3	N	11	THR	4.1
3	N	106	LEU	4.1
3	N	134	THR	4.0
3	O	195	SER	3.9
2	I	147	LEU	3.9
3	N	138	THR	3.8
3	N	82	THR	3.8
2	F	151	VAL	3.8
3	O	206	GLU	3.8
3	N	123	PRO	3.8
3	N	107	THR	3.7
3	N	179	SER	3.7
3	N	147	VAL	3.7
1	C	303	ALA	3.7
2	F	164	ASN	3.6
2	F	149	CYS	3.6
3	N	140	THR	3.6
3	O	197	GLN	3.6
1	C	239	ARG	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	340	HIS	3.4
2	F	180	GLN	3.4
2	F	167	SER	3.3
2	F	175	PHE	3.3
2	F	130	VAL	3.3
3	O	135	LEU	3.3
2	I	25	SER	3.3
3	O	205	VAL	3.2
2	I	145	VAL	3.2
2	I	191	THR	3.2
3	N	121	PHE	3.2
3	O	120	LEU	3.2
2	I	146	THR	3.2
2	I	192	VAL	3.1
3	N	124	SER	3.1
3	O	117	SER	3.1
2	G	135	PRO	3.1
2	I	198	PRO	3.1
2	I	197	TRP	3.0
3	N	111	GLN	3.0
2	J	136	GLY	3.0
3	N	19	THR	3.0
3	N	163	GLU	2.9
2	F	163	TRP	2.9
3	O	113	LYS	2.9
1	D	304	GLY	2.9
2	F	171	GLY	2.9
3	O	136	VAL	2.9
2	I	41	HIS	2.8
3	N	143	TYR	2.8
3	N	12	THR	2.8
3	M	14	PRO	2.8
2	G	11	LEU	2.8
2	G	167	SER	2.8
3	N	171	SER	2.8
3	O	121	PHE	2.8
3	N	10	LEU	2.8
2	I	133	LEU	2.8
2	F	172	VAL	2.8
3	K	149	VAL	2.8
3	N	137	CYS	2.8
2	I	173	HIS	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	F	152	LYS	2.8
3	N	80	ALA	2.7
2	F	156	PRO	2.7
2	F	133	LEU	2.7
3	N	18	VAL	2.7
2	H	43	LYS	2.7
3	N	169	LYS	2.7
2	F	174	THR	2.7
3	N	115	SER	2.6
1	D	80	THR	2.6
1	C	300	ILE	2.6
3	N	110	GLY	2.6
3	K	121	PHE	2.6
3	O	138	THR	2.6
2	G	86	LEU	2.6
2	F	216	ASP	2.6
2	J	195	SER	2.6
2	I	7	SER	2.5
3	N	167	PRO	2.5
1	B	308	TRP	2.5
2	I	124	LYS	2.5
2	I	212	SER	2.5
3	L	203	HIS	2.5
2	I	24	ALA	2.4
3	N	112	PRO	2.4
1	D	68	VAL	2.4
2	I	213	THR	2.4
2	I	194	SER	2.4
2	F	128	PRO	2.4
2	I	172	VAL	2.4
2	G	169	SER	2.4
2	I	187	SER	2.4
3	K	151	TRP	2.4
2	I	201	THR	2.4
3	N	168	SER	2.4
3	O	109	LEU	2.4
2	I	3	GLN	2.4
3	N	145	GLY	2.3
3	O	116	PRO	2.3
2	I	190	VAL	2.3
3	N	164	THR	2.3
2	J	134	ALA	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	I	196	THR	2.3
1	B	303	ALA	2.3
2	G	118	LEU	2.3
2	F	169	SER	2.3
3	N	114	SER	2.3
2	G	220	VAL	2.3
2	F	129	SER	2.3
2	G	175	PHE	2.3
3	K	136	VAL	2.3
3	N	116	PRO	2.3
1	D	338	PHE	2.3
3	O	177	ALA	2.3
3	K	81	GLN	2.3
1	C	338	PHE	2.3
2	I	221	PRO	2.3
3	N	166	GLN	2.3
2	I	125	THR	2.3
2	I	178	VAL	2.3
3	N	125	SER	2.3
2	G	18	MET	2.2
2	G	12	VAL	2.2
1	E	338	PHE	2.2
2	G	119	THR	2.2
3	N	77	ILE	2.2
3	O	131	ASN	2.2
1	C	1	SER	2.2
3	O	198	VAL	2.2
1	C	307	GLU	2.2
2	I	4	LEU	2.2
2	F	165	SER	2.2
3	N	117	SER	2.2
1	C	302	ASN	2.2
3	N	113	LYS	2.2
2	I	94	TYR	2.2
3	O	145	GLY	2.2
2	J	130	VAL	2.2
3	N	119	THR	2.2
2	G	134	ALA	2.1
2	J	135	PRO	2.1
2	I	1	GLU	2.1
2	J	206	VAL	2.1
3	M	69	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
3	N	146	VAL	2.1
3	N	177	ALA	2.1
2	F	173	HIS	2.1
3	O	82	THR	2.1
3	N	85	GLU	2.1
2	J	147	LEU	2.1
2	I	171	GLY	2.1
2	F	206	VAL	2.0
3	O	144	PRO	2.0
1	E	14	TYR	2.0
2	I	26	GLY	2.0
2	G	187	SER	2.0
3	N	183	LEU	2.0
3	O	175	TYR	2.0
1	B	309	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

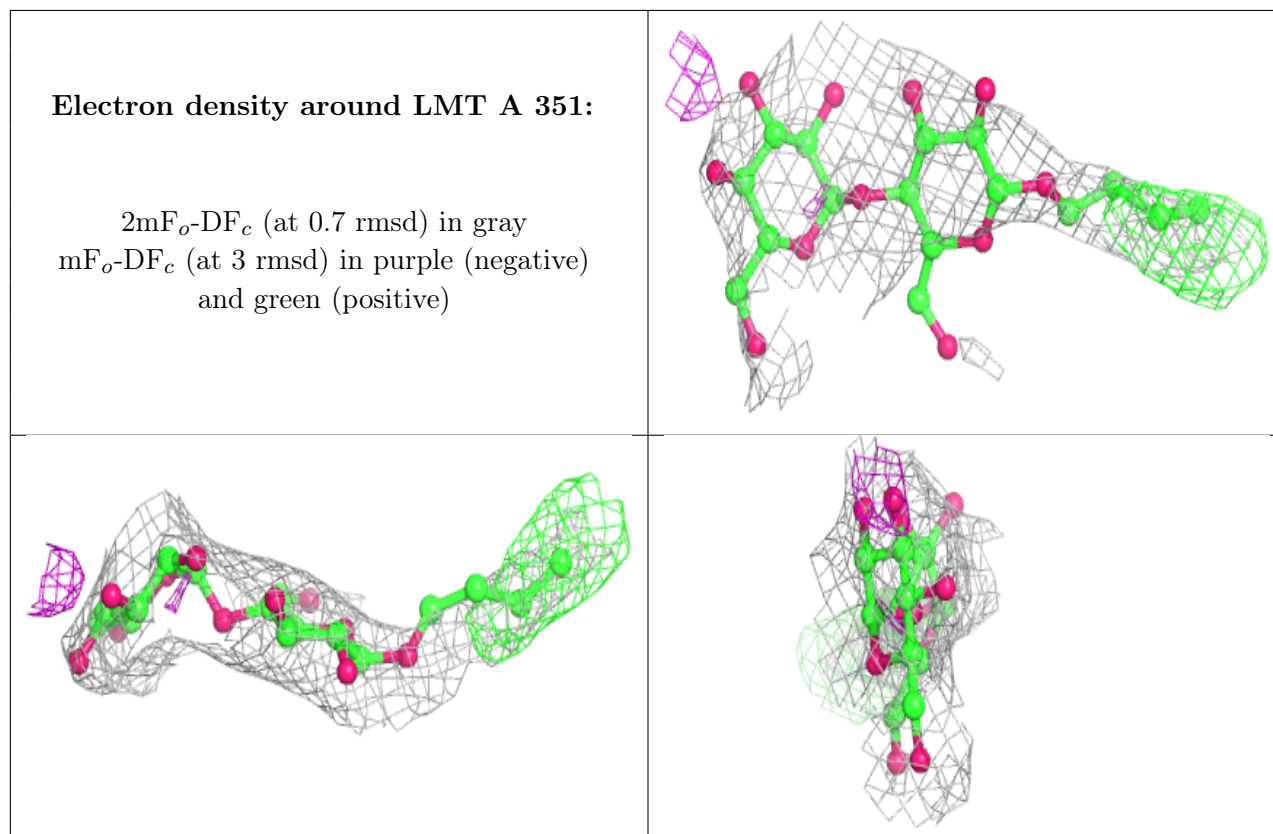
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	LMT	A	351	27/35	0.56	0.49	152,152,152,152	0
5	LMT	B	350	26/35	0.71	0.46	176,176,176,176	0
6	NAG	E	400	14/15	0.74	0.32	163,171,176,176	0
7	OCT	D	350	8/8	0.75	0.57	79,79,79,79	0
7	OCT	E	350	8/8	0.75	0.56	76,76,76,76	0
8	UND	B	352	11/11	0.77	0.42	74,74,74,74	0
6	NAG	C	400	14/15	0.84	0.19	128,130,131,132	0
6	NAG	B	400	14/15	0.85	0.48	123,124,129,130	0

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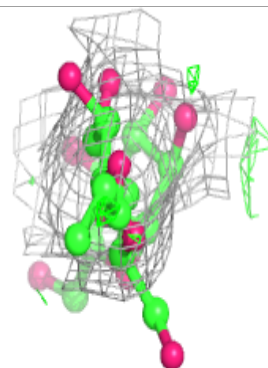
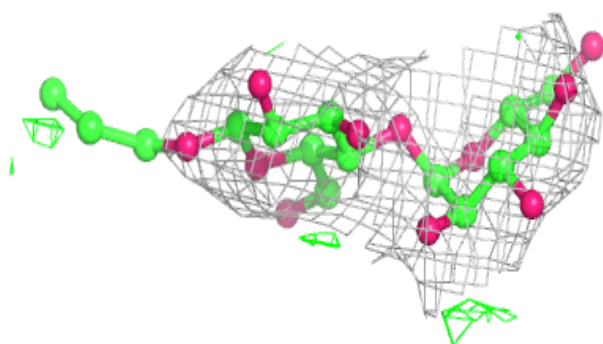
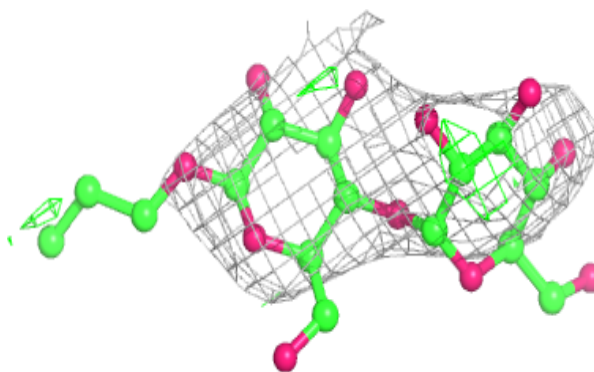
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	LMT	A	350	26/35	0.86	0.29	111,111,111,111	0
7	OCT	B	351	8/8	0.87	0.40	68,68,68,68	0
10	RI5	E	351	21/21	0.88	0.27	213,213,213,213	0
4	IVM	D	349	62/62	0.89	0.28	69,77,96,97	0
4	IVM	C	350	62/62	0.90	0.32	60,73,95,98	0
4	IVM	E	349	62/62	0.91	0.32	73,81,101,103	0
4	IVM	B	349	62/62	0.91	0.23	54,62,79,80	0
4	IVM	A	349	62/62	0.92	0.26	68,76,101,105	0
9	CL	C	349	1/1	0.96	1.04	76,76,76,76	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

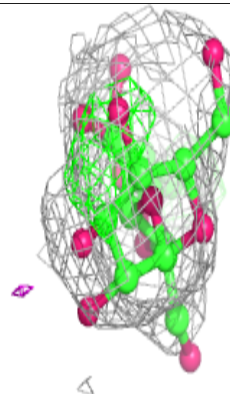
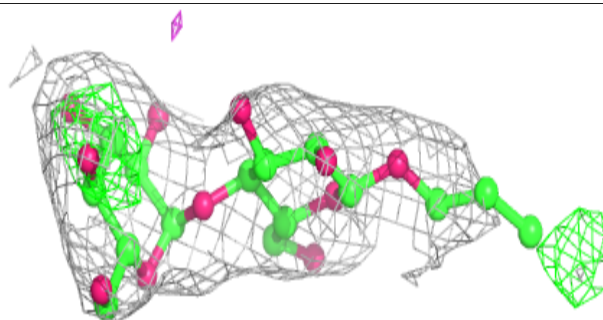
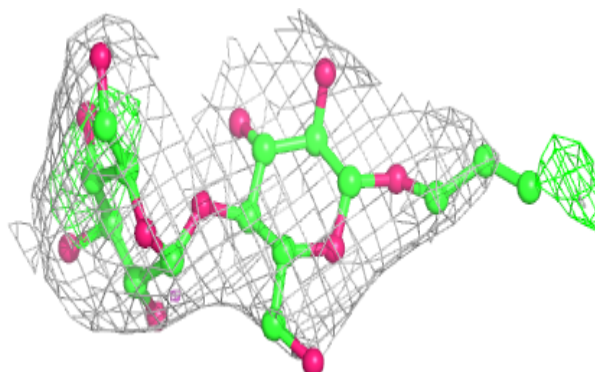


**Electron density around LMT B 350:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

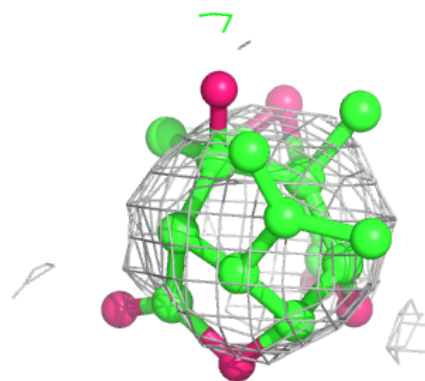
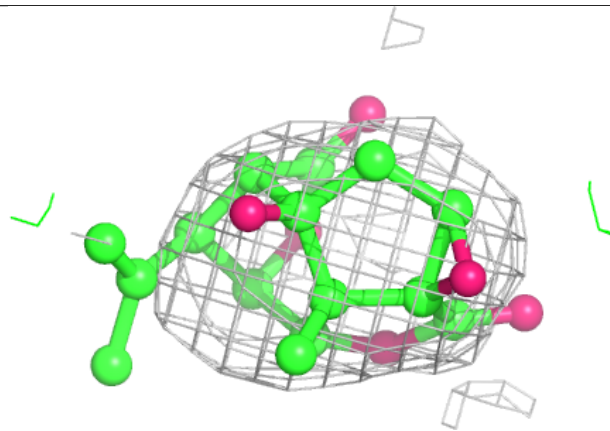
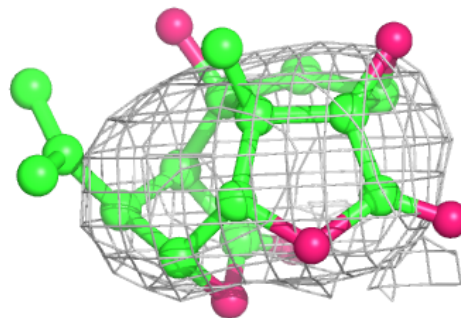
**Electron density around LMT A 350:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



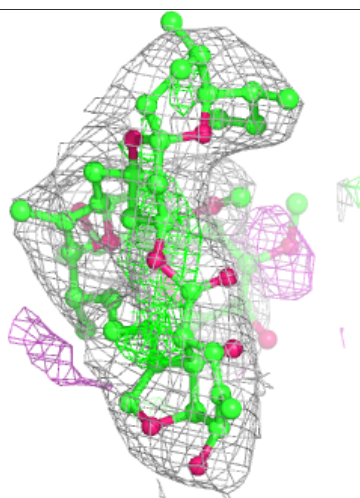
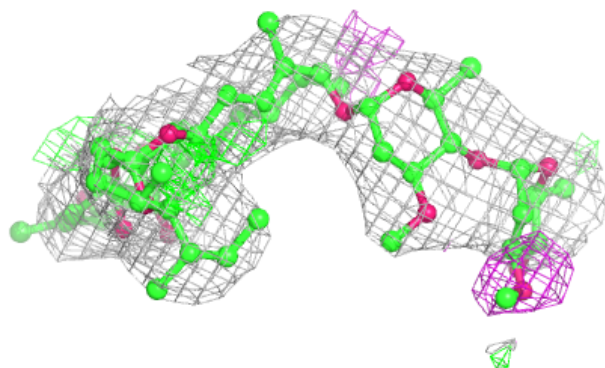
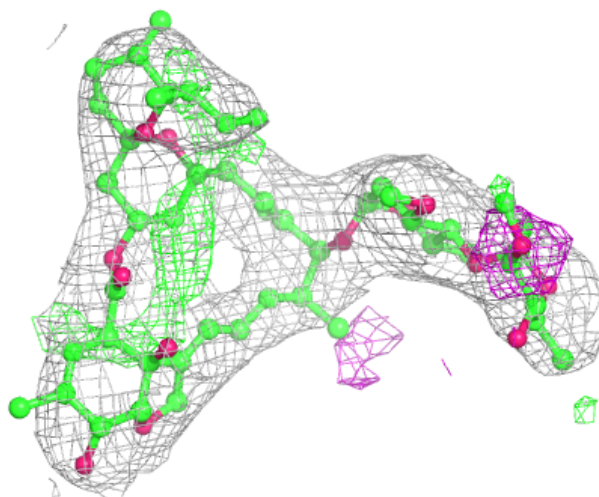
**Electron density around RI5 E 351:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around IVM D 349:**

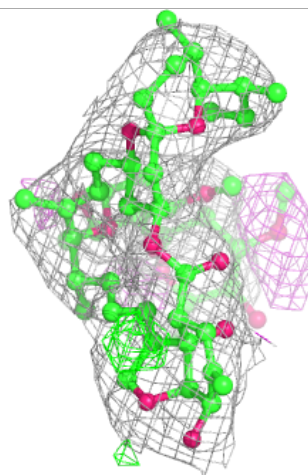
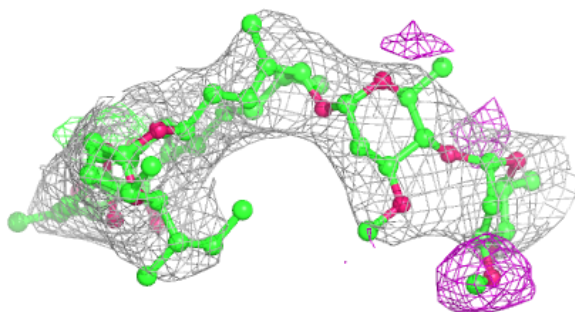
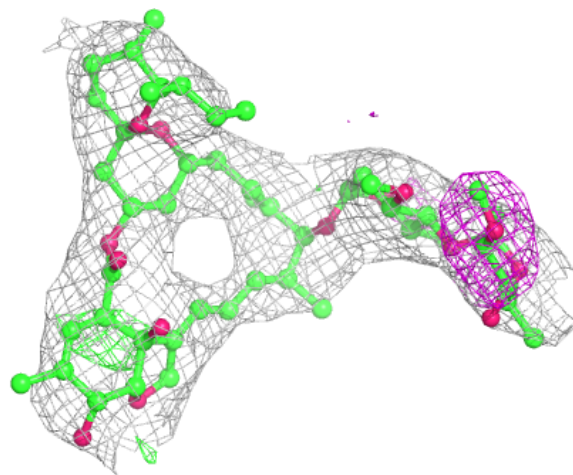
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





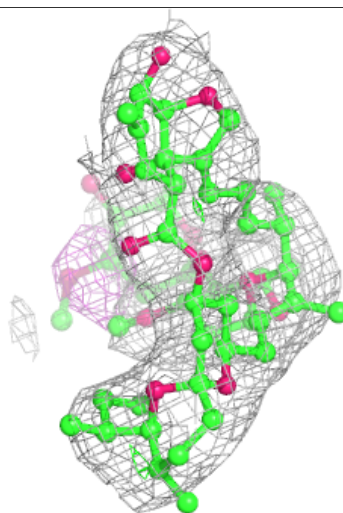
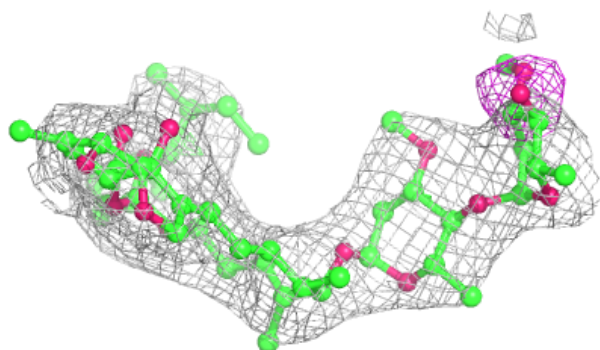
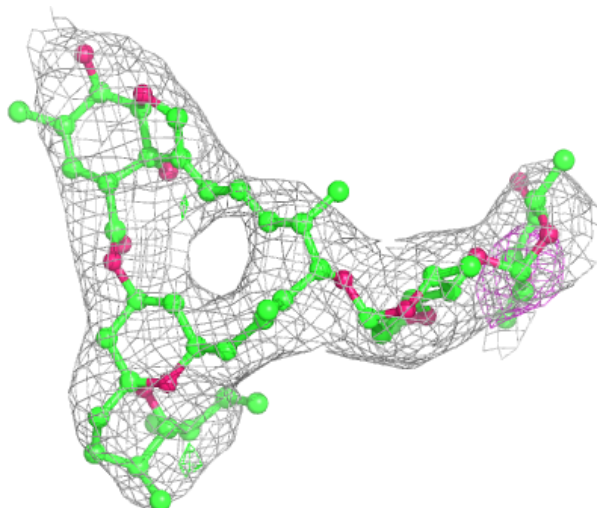
**Electron density around IVM C 350:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



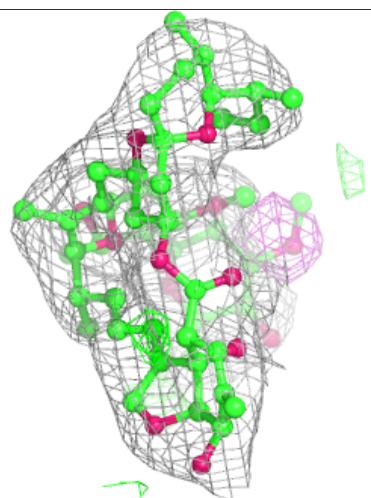
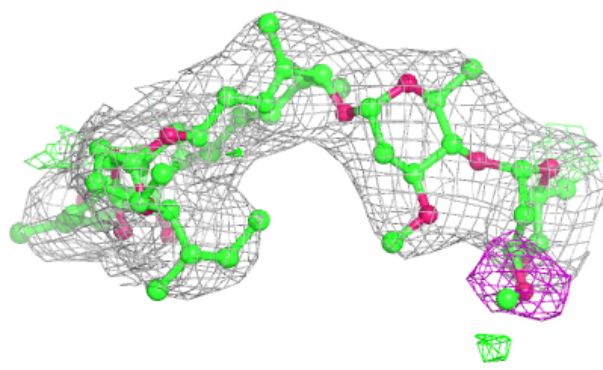
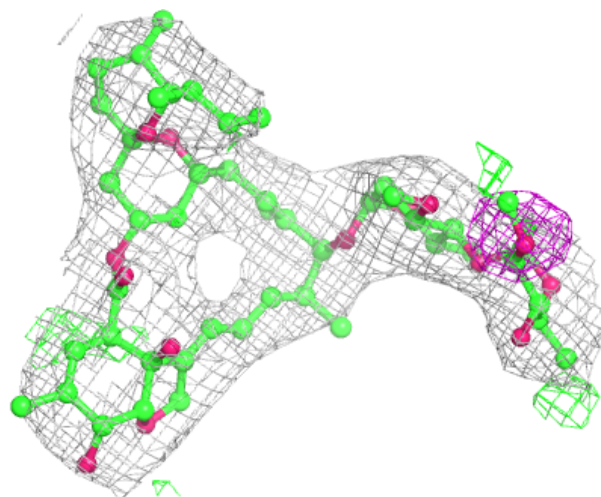
**Electron density around IVM E 349:**

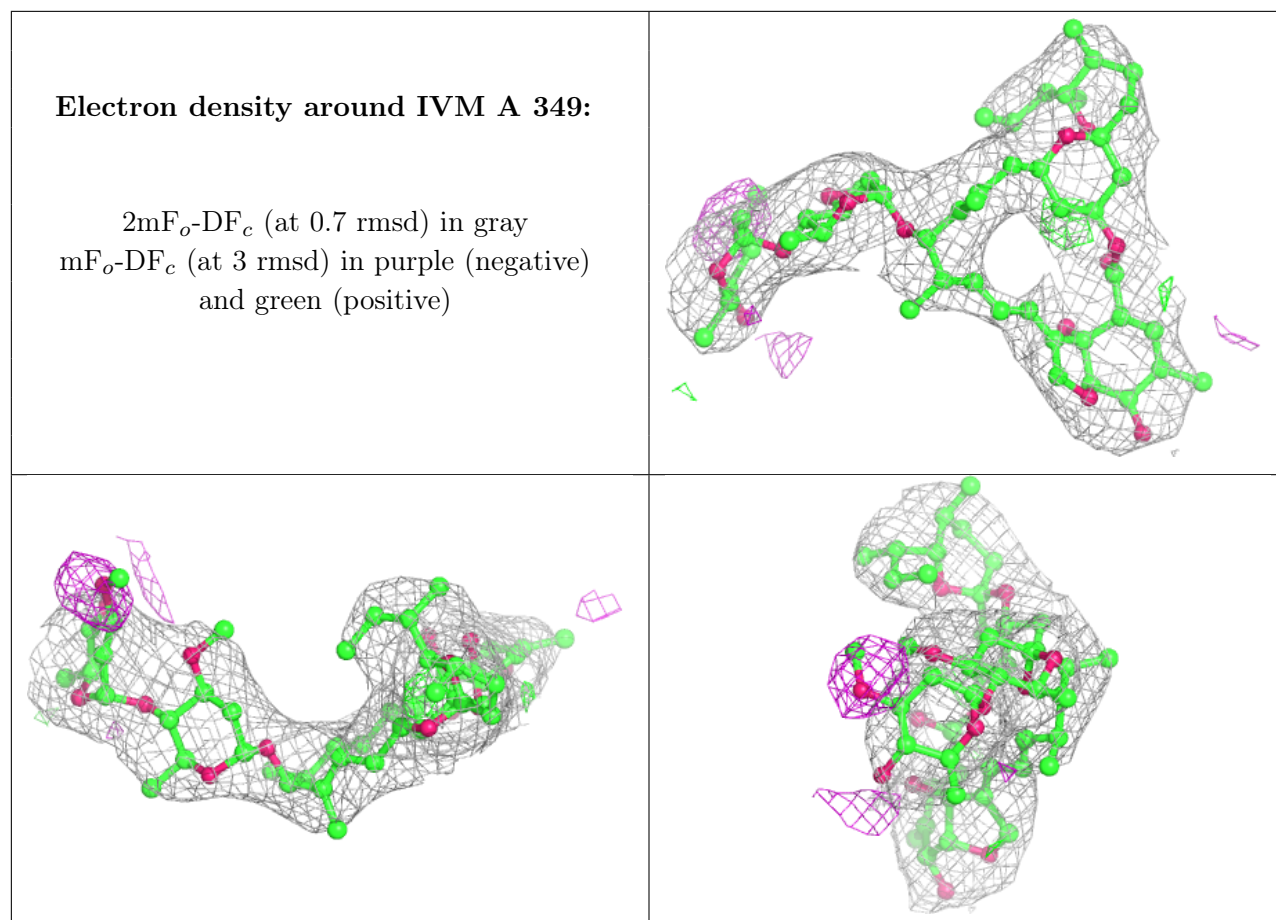
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around IVM B 349:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.